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Métodos matemáticos en problemas de entrelazamiento:
convertibilidad de estados, medidas conjuntas y halmiltonianos en PEPS

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Tesis Doctoral

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Introducción.

El interés del ser humano por la descripción de los fenómenos naturales ha sido siempre el principal motor de la ciencia. Una de las teorías más recientes de aquellas con las que podemos contar hoy es la Mecánica Cuántica, cuyo comienzo data de finales del siglo XIX y principios del siglo XX. Desde entonces, el desarrollo de esta teoría ha experimentado grandes avances, llevando a múltiples implicaciones teóricas y aplicaciones prácticas.

Esta tesis está relacionada con varios problemas relativos a una de las propiedades más importantes de la Mecánica Cuantica, el entrelazamiento, y con algunos de los objetos matemáticos con los que se intenta describir el papel del entrelazamiento en sistemas de materia condensada, los llamados *Projected Entangled Pair States*. Los problemas que resolvemos provienen de diferentes preguntas, relacionadas con cuestiones fundacionales, protocolos cuánticos y sistemas cuánticos de muchas partículas. ¿Qué tipo de estados se pueden conseguir a partir de otro dado en dos laboratorios distantes que sólo pueden comunicarse clásicamente? ¿Cual es la relación entre la incertidumbre ligada a las medidas cuánticas y las correlaciones no clásicas que pueden aparecer entre los resultados de las medidas? Y, finalmente, ¿cuál es la relación entre estados y hamiltonianos en el problema de clasificación de fases cuánticas de la materia?

Las técnicas matemáticas que usamos para resolver cada uno de los problemas que abordamos son muy diversos: bases simétricas en espacios de Banach, espacios invariantes por reordenamiento, programación semidefinida, teoría espectral de operadores autoadjuntos acotados y no acotados, etc. Obtenemos diversos resultados destacables, tanto en el ámbito de la Física como en el de las Matemáticas, algunos de los cuales ya han sido publicados en revistas internacionales.

La memoria está dividida en un resumen en español y la tesis completa en inglés. El resumen en español consta de esta introducción, la exposición de objetivos, herramientas y resultados, y una última parte de conclusiones y posibles futuras líneas de investigación. La tesis en inglés está a su vez dividida en introducción, un capítulo en el que introducimos el formalismo cuántico en términos de espacios de Hilbert, cuatro capítulos con los cuatro problemas que tratamos, conclusiones y bibliografía.

El primer problema al que nos enfrentamos surge del estudio de qué estados cuánticos pueden transformarse en otros en dos sitios alejados usando únicamente operaciones locales, comunicación clásica y algunos recursos adicionales, fundamentalmente catalizadores. El sistema cuántico resultante de considerar conjuntamente dos sistemas está descrito por el producto tensorial de esos dos sistemas. Y en el estudio de estas relaciones entre estados intervienen propiedades de simetría y multiplicatividad, lo que nos lleva a la siguiente pregunta en términos matemáticos: dados dos espacios X e Y, con bases simétricas $\{x_i\}_{i=1}^{\infty}$ e $\{y_i\}_{i=1}^{\infty}$ respectivamente, ¿qué condiciones ha de cumplir una norma tensorial

α para que la base producto $\{x_i \otimes y_j\}_{i,j=1}^{\infty}$ sea una base simétrica del espacio $X\hat{\otimes}_\alpha Y$? En un contexto más general, nos hacemos la pregunta análoga en espacios invariantes por reordenamiento: dados dos espacios invariantes por reordenamiento X e Y, y una norma tensorial α, ¿en qué casos tenemos que el espacio $X\hat{\otimes}_\alpha Y$ tiene también cierta estructura de invariancia por reordenamiento? Una descripción detallada del problema, su relación con el problema de convertibilidad de estados, y la resolución del problema obteniendo una caracterización de los espacios ℓ_p y c_0, y de los espacios L_p, están descritos en el capítulo 3.

En segundo lugar, caracterizamos las medidas que se pueden realizar simultáneamente. Desde que Heisenberg estableció el conocido Principio de Incertidumbre, es bien sabido que hay ciertas magnitudes que no se pueden determinar conjuntamente con precisión: cuanto más exacta se intente medir una de las magnitudes, más difuso será el resultado de la medición de la otra magnitud. En el caso de medidas proyectivas la solución depende de la conmutatividad de los observables asociados a la medida. Sin embargo, en el caso de medidas generalizadas no se había obtenido ninguna condición más allá del caso de *qubits*. Nosotros damos una caracterización computable para el caso más general de dos medidas dicotómicas cualesquiera, en términos de las correlaciones cuánticas que esas medidas pueden mostrar, mediante el cálculo de la máxima violación posible de las desigualdades de Bell que se pueden construir si una de las partes implicadas usa esas medidas. Este resultado establece una relación entre dos consecuencias fundamentales de la Mecánica Cuántica: el Principio de Incertidumbre y la no localidad. Algunas herramientas matemáticas que usamos para resolver esta pregunta son las formas primal y dual de la programación semidefinida y argumentos de convexidad. Además, estudiamos también la medibilidad conjunta de varias medidas dicotómicas, y de medidas no dicotómicas. El cuarto capítulo detalla los contenidos y resultados relacionados con este problema.

Por último, pasamos de problemas en sistemas de dos partes a problemas de sistemas en muchas partes, en concreto el de la relación entre estados y hamiltonianos. Los hamiltonianos son los observables que describen la energía de los sistemas y determinan cómo éstos evolucionan a lo largo del tiempo, y están determinados por las interacciones existentes en estos sistemas. Los efectos cuánticos son apreciables en un sistema cuando éste está a una temperatura muy baja, y a temperatura cero el sistema se estabiliza en los llamados estados fundamentales o *ground states*, que se corresponden con los autovectores asociados al menor autovalor del hamiltoniano. Es en estos estados en los que se pueden realizar medidas y observar las propiedades físicas del sistema. Cuando la temperatura es prácticamente nula pero no es cero, los estados de baja energía, o excitaciones de baja energía, también tienen un papel importante en la descripción del sistema. La relación entre hamiltonianos y ground states nos lleva a la siguiente pregunta: dado un estado cuántico, ¿se pueden conseguir diferentes hamiltonianos con distintas propiedades que tengan al estado como estado fundamental? El tipo de estados para los cuales estudiamos este problema son los llamados Projected Entangled Pair States o PEPSs, firmes candidatos a describir la física que aparece en sistemas con interacciones locales. Estos estados tienen un hamiltoniano asociado de forma natural, el hamiltoniano *parent* o parental, de cuya construcción estudiamos la robustez: ¿llevan pequeñas perturbaciones de la descripción tensorial de los PEPSs a pequeñas perturbaciones de los hamiltonianos parent asociados? Los casos que estudiamos son los de PEPSs unidimensionales, o Matrix Product States (MPSs), y PEPSs dos-dimensionales, en el primer caso de forma general y en el segundo mostrando el comportamiento para el ejemplo más conocido, el código tórico de Kitaev.

En el caso de MPSs (capítulo 5) mostramos en qué casos la construcción es robusta para perturbaciones de las matrices que definen el estado, y, cuando no lo es, construimos una nueva familia de hamiltonianos, los hamiltonianos *uncle* o *avunculares*, como el límite de los hamiltonianos parent cuando la perturbación se anula. Además, estudiamos propiedades de estos hamiltonianos uncle, como el espacio de estados fundamentales y el espectro. Demostramos que el hamiltoniano uncle tiene el mismo conjunto de estados fundamentales que el hamiltoniano parent, y que no presenta *gap* espectral. Esto contrasta con el hecho de que el hamiltoniano parent siempre tiene gap. En el caso del código tórico construimos también un hamiltoniano uncle para una perturbación concreta, obteniendo resultados similares respecto al conjunto de estados fundamentales y la comparativa de los espectros (capítulo 6). Para llegar a estos resultados usamos principalmente resultados espectrales de operadores autoadjuntos acotados y no acotados, relacionando para ello los espectros de sistemas con un número finito de partículas con los de sistemas de infinitas partículas.

Por último, recogemos las principales conclusiones que se pueden derivar de los resultados obtenidos, junto con una breve exposición de problemas relacionados para próximos trabajos.

Sobre esta tesis.

Esta memoria de tesis doctoral es presentada por Carlos Fernández González, en el Departamento de Análisis Matemático de la Universidad Computense de Madrid, para optar al título de Doctor en Matemáticas, con Mención Europea. El trabajo ha sido dirigido por el profesor David Pérez García, en el Programa de Doctorado Matemáticas de la Facultad de Matemáticas de la misma universidad.

La tesis consta de una amplia introducción en español, de las páginas 7 a 36, y de la tesis completa en ingles. El resumen en inglés está incorporado en la introducción de la misma.

Durante el periodo doctoral, el doctorando ha realizado dos estancias de investigación, en el Instituto Niels Bohr de Copenhagen con el profesor Michael M. Wolf, del 15 de septiembre al 15 de diciembre de 2008, y en el Instituto de Información Cuántica de la universidad RWTH en Aachen con el profesor Norbert Schuch, del 1 de febrero al 1 de mayo de 2013. El trabajo presentado ha sido parcialmente realizado durante dichas estancias.

Parte del trabajo ha sido también realizado durante el Workshop en Información Cuántica que tuvo lugar en el mes de junio de 2011 en el Centro de Ciencias de Benasque Pedro Pascual.

Este trabajo ha sido parcialmente financiado por la beca-contrato FPU del MCE y el contrato de ayudante de la UNED de los que ha disfrutado el doctorando, así como por los proyectos MTM 2004-08080-C02-01 y MTM 2008-01366 del MICINN, el proyecto MTM 2011-26912 del MINECO, el proyecto QUITEMAD de la Comunidad de Madrid, el proyecto europeo CHIST-ERA CQC (financiado parcialmente por el proyecto PRI-PIMCHI-2011-1071 del MINECO), y el programa de movilidad Puentes Internacionales de la UNED.

El trabajo que recoge esta memoria ha sido parcialmente publicado en revistas internacionales de alto impacto con revisión por pares. Tres artículos han sido aceptados, comprendiendo respectivamente los contenidos principales de los capítulos 3, 4 y 6:

> C. Fernández-González, C. Palazuelos y D. Pérez-García, *The natural rearrangement invariant structure on tensor products*, Journal of Mathematical Analysis and Applications **343** 1, 40-47 (2008).
>
> M. M. Wolf, D. Pérez-García y C. Fernandez, *Measurements incompatible in Quantum Theory cannot be measured jointly in any other local theory*, Physical Review Letters **103**, 230402 (2009), arXiv:quant-ph/0905.2998.
>
> C. Fernández-González, N. Schuch, M. M. Wolf, J. I. Cirac y D. Pérez-García, *Gapless Hamiltonians for the Toric Code Using the Projected Entangled Pair State Formalism*, Physical Review Letters **109**, 260401 (2012), arXiv:quant-ph/1111.5817.

Los contenidos principales del capítulo 5 han sido enviados para su publicación en la revista Communications in Mathematical Physics, habiendo recibido unos primeros informes positivos sobre su posible aceptación.

La mayor parte de los resultados han sido presentados en distintos congresos.

Contribuciones orales:

> *La estructura natural de espacio invariante por reordenamiento sobre el producto tensorial*, presentado en el IV Encuentro de Análisis Funcional y Aplicaciones, Salobreña (Granada), España, 2008. Presentado por C. Palazuelos, trabajo conjunto con C. Fernández-González y D. Pérez-García.
>
> *Measurements incompatible in quantum theory cannot be measured jointly in any other no-signaling theory*, presentado en el 13th Workshop on Quantum Information Processing, QIP2010, Zürich, Suiza, 2010. Presentado por M. M. Wolf, trabajo conjunto con D. Pérez-García y C. Fernández-González.
>
> *Sistemas cuánticos: límite termodinámico y operadores no acotados*, presentado en el VII Encuentro de Análisis Funcional y Aplicaciones, Jaca (Huesca), España, 2011. Presentado por C. Fernández-González, trabajo conjunto con N. Schuch, M. M. Wolf, J. I. Cirac y D. Pérez-García.
>
> *Gapless Hamiltonians for non-injective Matrix Product States*, presentado en Networking tensor networks: many-body systems and simulations, Benasque (Huesca), España, 2012. Presentado por C. Fernández-González, trabajo conjunto con N. Schuch, M. M. Wolf, J. I. Cirac y D. Pérez-García.

Gapless Hamiltonians for non-injective PEPS, presentado en el Benasque Symposium on Topological Quantum Information, Benasque (Huesca), España, 2013. Presentado por C. Fernández-González, trabajo conjunto con N. Schuch, M. M. Wolf, J. I. Cirac y D. Pérez-García.

Presentaciones de póster:

Gapless Hamiltonians for the toric code using the PEPS formalism, presentado en el 16th Workshop on Quantum Information Processing, QIP2013, Beijing, China, 2013. Trabajo de C. Fernández-González, N. Schuch, M. M. Wolf, J. I. Cirac y D. Pérez-García.

Objetivos, herramientas y resultados.

Este capítulo recoge los principales contenidos de la tesis, los problemas que hemos tratado, las herramientas usadas, los objetivos perseguidos y los resultados obtenidos.

Espacios invariantes por reordenamiento en productos tensoriales.

Motivación. A la hora de estudiar ciertos problemas en información cuántica, es necesario establecer el paradigma en el que se va a trabajar, dependiendo de los recursos disponibles, el tipo de comunicación permitida, etc. ¿Se considerará el problema admitiendo que se puede almacenar una cantidad ilimitada de datos, o se limitará esta cantidad a cierto valor? ¿Se permitirá comunicación cuántica, únicamente clásica, cierta comunicación condicionada por las fases del protocolo, etc.? ¿Compartirán las distintas partes envueltas en el problema recursos cuánticos, o quizás aleatoriedad compartida? De estas preguntas y muchas otras dependen las características de los problemas que se quieran estudiar.

Entre estos distintos escenarios, ha destacado el llamado "operaciones locales y comunicación clasica" (LOCC, de sus siglas en inglés), debido a la gran similitud con las posibilidades reales de dos laboratorios (o partes) distantes entre sí. Dados dos sistemas A y B que representen las dos partes distantes, usualmente llamadas Alicia y Benito (o Alice y Bob), únicamente se pueden realizar operaciones cuánticas locales, en A o en B, y por tanto no se permiten operaciones globales en el sistema compuesto $A \otimes B$. Este tipo de operaciones son del tipo $U \otimes \mathbb{I}$ y $\mathbb{I} \otimes V$ (o $U \otimes V$) para el caso de evoluciones unitarias, y las medidas pueden ser igualmente descritas por productos $\{P_i \otimes Q_j\}_{i,j}$, donde $\{P_i\}_i$ y $\{Q_j\}_j$ deben ser medidas en el sistema de Alicia y en el sistema de Benito respectivamente. La otra característica del escenario LOCC es que se permite la transmisión ilimitada de información clásica (es decir, se pueden transmitir tantos *bits* como se quiera), en tantas rondas de comunicación como se desee, pero ningún estado cuántico puede ser transmitido entre Alicia y Benito.

Una vez fijadas las condiciones, un problema muy importante, en el que el entrelazamiento juega un papel crucial, es el siguiente: dado un estado compartido por Alicia y Benito, ¿qué otros estados pueden obtener a partir de él? Esta pregunta en el paradigma LOCC ha sido el origen de dos de las medidas de entrelazamiento más estudiadas: el entrelazamiento de formación y el entrelazamiento destilable. La primera está relacionada con cuántas copias de pares EPR o estados bipartitos máximamente entrelazados (por ejemplo, $|00\rangle + |11\rangle)/\sqrt{2})$ se necesitan para crear un estado dado usando únicamente LOCC, mientras que la segunda está determinada por la operación inversa, por cuántos pares EPR se pueden obtener de un estado dado. Ambas medidas se estudian en el caso asintótico, como el límite del cociente entre el número de pares EPR necesitados u obtenidos y el número n de copias del estado considerado.

Estas medidas de entrelazamiento y la convertibilidad LOCC surgen de ver el entrelazamiento como un recurso para ciertos protocolos de comunicación. Los pares EPR permiten realizar algunas operaciones que no son posibles usando únicamente recursos clásicos, como la teleportación cuántica [**16**], la distribución cuántica de claves [**38**], la codificación superdensa [**18**] o el diseño de mejores estrategias en juegos cooperativos [**65, 69**]. Consecuentemente, si un estado puede ser convertido en otro mediante LOCC, el primero es más útil que el segundo y está más entrelazado.

El problema ha sido ampliamente estudiado en el caso de estados puros bipartitos. En primer lugar, aunque el paradigma LOCC permite tantas rondas de comunicación como se quiera, el resultado es el mismo si únicamente se permite una ronda de comunicación [**78**]. La caracterización matemática de la convertibilidad LOCC fue probada por Nielsen en [**90**], demostrando que la clave está en los autovalores de las matrices de densidad reducidas de los estados. Dados dos estados $|\varphi_1\rangle, |\varphi_2\rangle \in A \otimes B$, cuyas matrices de densidad reducidas tienen como autovalores $\bar{\lambda} = (\lambda_1, \ldots, \lambda_n)$ y $\bar{\mu} = (\mu_1, \ldots, \mu_n)$ respectivamente, es posible transformar $|\varphi_1\rangle$ en $|\varphi_2\rangle$ usando LOCC si y sólo si $\bar{\lambda}$ está mayorado por $\bar{\mu}$ (o $\bar{\mu}$ mayora a $\bar{\lambda}$):

$$\sum_{i=1}^{k} \lambda_i^* \leq \sum_{i=1}^{k} \mu_i^*, \ \forall k$$

donde los vectores $\bar{\lambda}^*$ y $\bar{\mu}^*$ denotan los reordenamientos decrecientes de $\bar{\lambda}$ y $\bar{\mu}$. Esta posibilidad de convertibilidad se expresa como $|\varphi_1\rangle \to |\varphi_2\rangle$.

Este tipo de convertibilidad presenta algunos casos sorprendentes. Jonathan y Plenio [**64**] mostraron que puede darse el caso de que un estado $|\varphi_1\rangle$ no pueda ser convertido en otro estado $|\varphi_2\rangle$, y sin embargo exista un tercer estado $|c\rangle \in A \otimes B$, llamado catalizador, que permita tal conversión: $|\varphi_1\rangle \otimes |c\rangle \to |\varphi_2\rangle \otimes |c\rangle$. El catalizador ha de estar necesariamente entrelazado para que esto pueda llegar a suceder, por lo que este tipo de convertibilidad recibe el nombre de LOCC asistido por entrelazamiento o ELOCC.

Por otro lado, Bandyopadhyay, Roychowdhury y Sun [**14**] probaron que también puede darse el caso de que un estado $|\varphi_1\rangle$ no se pueda convertir en otro estado dado $|\varphi_2\rangle$, pero que cierto número finito de copias del primero, $|\varphi_1\rangle^{\otimes n}$, sí pueda ser convertido en el mismo número finito de copias del segundo. Este problema es llamado convertibilidad MLOCC, por el uso de multiples copias de los estados.

En [**10**] Aubrun y Nechita dieron una caracterización matemática de ambos problemas: $|\varphi_1\rangle$ puede ser "casi" convertido en $|\varphi_2\rangle$ usando MLOCC o ELOCC si y sólo si se tiene que $\|\bar{\lambda}\|_p \leq \|\bar{\mu}\|_p, \ \forall p \geq 1$. El "casi" surge ante la posible necesidad de que los catalizadores tengan dimensión infinita, con lo que caracterizaron la adherencia de los estados que podrían ser conseguidos a partir de uno dado.

En estos últimos problemas, las propiedades de invariancia por reordenamiento de la convertibilidad LOCC han de presentarse en la base producto del producto tensorial, pues los autovalores de la matriz de densidad reducida de estados producto del tipo $|\varphi\rangle \otimes |c\rangle$ y

$|\varphi\rangle^{\otimes n}$, dada la partición definida por A y B, se obtienen como productos de los autovalores de los estados individuales. Este hecho nos lleva a plantearnos si estas condiciones de simetría y multiplicatividad son los únicos ingredientes necesarios para deducir la caracterización encontrada por Aubrun y Nechita del problema de las convertibilidades MLOCC y ELOCC. La pregunta que nos hacemos, por tanto, es la siguiente

> Dados dos espacios X e Y con base simétrica, ¿en qué casos la base producto de $X\hat{\otimes}_\alpha Y$ es simétrica para alguna *crossnorm* α?

En el caso en que la pregunta que previamente hemos hecho sobre las convertibilidades MLOCC y ELOCC tuviera una respuesta positiva, deberíamos obtener como respuesta a esta pregunta matemática la familia de espacios ℓ_p. En efecto, probamos que X e Y deben ser necesariamente el mismo espacio, que debe ser un espacio ℓ_p, con $1 \leq p < \infty$, o el espacio c_0, y que la norma α debe ser necesariamente la que hace al producto tensorial ser el mismo espacio, $\alpha = \Delta_p$ o $\alpha = \varepsilon$. Posteriormente, Aubrun y Nechita obtuvieron el mismo resultado en [**11**], usando el mismo tipo de técnicas que usaron para probar la caracterización de las convertibilidades MLOCC y ELOCC anteriormente mencionado.

En relación con este problema, nos planteamos también la pregunta análoga en el caso de espacios invariantes por reordenamiento sobre espacios de medida continuos. Por tanto, las principales herramientas matemáticas que usamos para estos problemas son las bases simétricas en espacios de Banach y los espacios invariantes por reordenameinto.

En contraste con estos resultados en el caso puro bipartito, en los casos mixto bipartito y puro multipartito no existen resultados tan concluyentes. Aún no se ha encontrado una descripción matemática sencilla de la convertibilidad LOCC, aunque hay resultados en esta dirección. Por ejemplo, Kraus caracterizó en [**70**] el conjunto de operaciones locales unitarias que clasifican el entrelazamiento multipartito puro (equivalencia LU), y que indican el mínimo conjunto de condiciones que deben permanecer invariantes bajo cualquier medida de entrelazamiento. Posteriormente, de Vicente et al. dieron una clasificación del entrelazamiento en estados puros de 3 qubits usando medidas de entrelazamiento operacionales, relacionando ésta con el escenario LOCC.

Otro problema que ha suscitado un gran interés, debido a la naturaleza probabilística inherente a la Mecánica Cuántica, es la conversión LOCC estocástica o SLOCC, que estudia el problema de cuándo un estado puede convertirse en otro con alguna probabilidad [**37**]. Vidal demostró que, en el caso de estados puros bipartitos y considerando copias únicas de los estados, la conversión depende únicamente del rango de la matrices de densidad reducidas de los estados [**132**], mostrando además una fórmula sencilla que da la máxima probabilidad de conversión. En el caso de estados mixtos, podemos destacar [**66, 75, 127, 128**], y en el caso puro tripartito [**28**], en el que se demuestra la complejidad *NP-hard* del problema conectándolo con ciertos problemas de complejidad algebraica. Esta conexión abre la puerta al uso de resultados en uno de los campos para la obtención de resultados en el otro.

Productos tensoriales y bases simétricas. Entre los primeros resultados estudiando el comportamiento de las bases producto en productos tensoriales, podemos encontrar el resultado de Gelbaum y Lamadrid [**48**], en que muestran que dados dos espacios X e

Y, con bases $\{x_n\}_{n=1}^{\infty}$ e $\{y_m\}_{m=1}^{\infty}$, la base producto $\{x_n \otimes y_m\}_{n,m=1}^{\infty}$, con determinado orden entre los elementos de la base, es una base de la compleción del espacio $X \otimes_\alpha Y$ para cualquier crossnorm uniforme α.

Otro resultado muy importante en este contexto es el teorema de Pisier-Schütt, probado independientemente por ambos autores en [**106**] y [**118**]. Una versión débil del mismo es la siguiente: dados dos espacios con base incondicional, la compleción de su producto tensorial respecto a una norma tensorial tiene también una base incondicional si y sólo si la base producto es incondicional.

Mientras que la incondicionalidad en productos tensoriales ha despertado gran interés, hay escasos resultados en el estudio de bases simétricas en estos productos. Los únicos resultados que conocemos son debidos a Schütt [**117**] y Read [**108**]. En el primero de ellos el autor demostró que la constante de simetría de los espacios $\ell_p^n \otimes_{\Delta_r} \ell_r^n$ no está acotada en la dimensión n para $1 \le p, r < 2,\ p \neq r$, y en el segundo se muestra un ejemplo de un espacio con base simétrica E y una crossnorm β para la que el espacio es isomorfo a $E \hat{\otimes}_\beta E$, diferente de los ya conocidos verificando esa propiedad, ℓ_p y c_0. Además, se prueba que E y $E \hat{\otimes}_\beta E$ no son isomorfos como retículos. $E \hat{\otimes}_\beta E$ denota la compleción de $(E \otimes E, \beta)$.

Productos tensorales y espacios invariantes por reordenamiento. Así como el problema que nos planteamos en términos de bases pregunta si la base producto es simétrica, no si existe alguna base simétrica en el espacio producto, la pregunta en el contexto más general de espacios invariantes por reordenamiento (r.i.) también tiene una formulación más específica que la de que el producto sea un espacio r.i. cualquiera: dados dos espacios r.i. $X(\Omega_1)$ y $Y(\Omega_2)$, ¿en qué casos tendremos que $X(\Omega_1) \hat{\otimes}_\alpha Y(\Omega_2) = Z(\Omega_1 \times \Omega_2)$ para algún espacio r.i. Z y alguna crossnorm α?

La conexión entre productos tensoriales y espacios de Banach ha sido estudiada en diversos trabajos, véase por ejemplo [**82, 93**] y las referencias citadas en ellos. El enfoque general ha sido el siguiente: dados $X(\Omega_1)$, $Y(\Omega_2)$ y $Z(\Omega_1 \times \Omega_2)$, ¿en qué casos el operador bilineal

$$B : X(\Omega_1) \times Y(\Omega_2) \longrightarrow Z(\Omega_1 \times \Omega_2),$$

definido como $B(x,y)(s,t) = x \otimes y(s,t) = x(s)y(t)$ para todo $(s,t) \in \Omega_1 \times \Omega_2$, es acotado? O, equivalentemente, ¿cuándo induce una inmersión continua $X(\Omega_1) \hat{\otimes}_\pi Y(\Omega_2) \subseteq Z(\Omega_1 \times \Omega_2)$? En esta pregunta, π es la norma tensorial proyectiva en $X(\Omega_1) \otimes Y(\Omega_2)$.

La relación de la continuidad del operador B y el problema de estabilidad de operadores integrales (ver [**82**], Part III) ha motivado un gran interés de este problema. La mayor parte de los trabajos (por ejemplo, [**5, 83, 84, 85, 93, 121**]) se han centrado en ciertos espacios importantes, como los espacios de Lorentz, de Orlicz o de Marcinkiewicz.

Más recientemente, en [**8**], el problema ha sido estudiado en el contexto de funciones simétricas en el intervalo [0,1], donde el producto tensorial es usado para estudiar el espacio multiplicador $\mathcal{M}(X)$ de X. En [**9**] los autores relacionan, en espacios r.i. sobre $[0,1]$, el espacio multiplicador con propiedades de los subespacios de X y, de nuevo, con la continuidad del operador B.

En principio, puede haber distintas estructuras r.i. en un espacio $X(\Omega_1)\hat{\otimes}_\alpha Y(\Omega_2)$, pero existe una estructura natural, sobre el espacio de medida $\Omega_1 \times \Omega_2$, asociada al operador producto B. La pregunta por tanto se plantea en estos términos, y nos interesamos por aquellos casos en que el operador B es un isomorfismo topológico (sobreyectivo).

Finalmente, existen otros problemas relacionando productos tensoriales y estructuras ordenadas. En **[45]** y **[46]** el autor se planteó la posibilidad de definir crossnorms en productos tensoriales de retículos de Banach que conservaran la estructura de retículo (véase también **[35]**). En esta dirección ha habido también bastantes más trabajos, aunque la estructura simétrica de los espacios r.i. hace nuestro problema más restrictivo.

Resultados principales. Para el problema en bases simétricas[1], el resultado que obtenemos se basa en una caracterización de los espacios ℓ_p y c_0 dada por Altshuler en **[3]**: dado un espacio X con base simétrica $\{e_i\}_{i=1}^\infty$, X es isomorfo a c_0 o algún ℓ_p si y sólo si para cualesquiera $a = \sum_{i=1}^\infty a_i e_i$ y $b = \sum_{j=1}^\infty b_j e_j$, $a, b \in X$, y cualquier conjunto de sucesiones disjuntas de la base $\{(e_{i,j})_{j=1}^\infty,\ i \in \mathbb{N}\}$, existe una constante $K > 0$ tal que

$$K^{-1}\|a\| \cdot \|b\| \leq \| \sum_{i,j=1}^\infty a_i b_j e_{i,j} \| \leq K\|a\| \cdot \|b\| \ .$$

Esta caracterización nos permite demostrar el primer resultado:

Teorema. *Si X e Y son espacios con bases simétricas $\{x_n\}_{n=1}^\infty$ y $\{y_n\}_{n=1}^\infty$ respectivamente, y existe una crossnorm α que haga $\{x_n \otimes y_m\}_{n,m=1}^\infty$ ser base simétrica del espacio $Z = X\hat{\otimes}_\alpha Y$, entonces $X = Y = Z$ es el espacio ℓ_p y $\alpha = \Delta_p$, para algún $1 \leq p < \infty$, o es el espacio c_0 y $\alpha = \varepsilon$.*

En la pregunta que nos hacemos relativa a espacios invariantes por reordenamiento usamos dos trabajos previos de Ashtaskin et al. en **[9]** y Hernández et al. en **[62]** para probar nuestro segundo resultado:

Teorema. *Sean X, Y y Z espacios r.i. sobre $\Omega = [0,1]$ or $[0,\infty)$, tales que el operador multiplicación*

$$B : X(\Omega) \otimes_\alpha Y(\Omega) \longrightarrow Z(\Omega \times \Omega),$$

definido como $B(x \otimes y)(s,t) = x(s)y(t)$ para todo $(s,t) \in \Omega \times \Omega$, es acotado. Entonces B puede extenderse a un isomorfismo topológico sobreyectivo $\hat{B}$ de $X(\Omega)\hat{\otimes}_\alpha Y(\Omega)$ en $Z(\Omega \times \Omega)$ si y sólo si existe algún valor $p \in [1,\infty)$ tal que $X = Y = Z = L_p$ y $\alpha = \Delta_p$.

También discutimos la optimalidad del primer resultado, en el sentido de que no puede existir un resultado del estilo del teorema de Pisier-Schütt en este contexto, mostrando que el espacio que dio Read en **[108]** y el espacio universal de Pełczyński para bases incondiconales **[99]** serían contraejemplos de un resultado en esa diercción junto con la

[1]Nótese que ℓ_∞ no tiene base, por lo que siempre que nos refiramos a algún ℓ_p será para $1 \leq< p < \infty$.

crossnorm β dada por Read en el mismo trabajo. Ambos son ejemplos de espacios X con base simétrica tales que $X\hat{\otimes}_\beta X$ tiene también base simétrica pero la base producto no es simétrica.

Medidas conjuntas y desigualdades de Bell.

Motivación. Una de las consecuencias más sorprendentes de la Mecánica Cuántica es la posible no localidad de la naturaleza, señalada por primera vez por Einstein, Podolki y Rosen en [**39**] en 1935. Si en dos lugares distantes se realizan ciertas medidas sobre estados entrelazados, los resultados obtenidos pueden llegar a mostrar correlaciones que no pueden ser explicadas con las leyes clásicas de la Física. Este comportamiento “mágico” fue entendido inicialmente como una falta de completitud de la teoría cuántica.

Sin embargo, cualquier teoría física que pueda ser un refinamiento de la Mecánica Cuántica ha de mostrar también este extraño comportamiento. Treinta años más tarde, Bell propuso un experimento [**15**] que podría llegar a certificar la existencia de tales correlaciones, y que por tanto daría evidencias que apoyarían la validez de la teoría cuántica. En su experimento, todo resultado proveniente de “comportamientos clásicos” debería estar acotado por cierto valor, que sin embargo sería sobrepasado por algún estado cuántico en caso de que estos existieran.

Tal prueba experimental, aún no habiendo sido efectuada con todas las garantías, es prácticamente dada por cierta, y quedan pocas dudas sobre la validez de la Mecánica Cuántica. El interés en la no localidad es también muy elevado en el campo de la información cuántica, debido a las aplicaciones a las que lleva este fenómeno, que abarcan desde la criptografía cuántica [**38, 104, 124**] a la amplificación de aleatoriedad [**31**], así como por sus implicaciones teóricas en los fundamentos de la Física.

No todo experimento cuántico sirve para mostrar distribuciones de probabilidad cuánticas. Por un lado, esto depende del estado bipartito sobre el que se realizan las medidas, ya que cualquier resultado obtenido usando estados separables, e incluso cierto tipo de estados entrelazados, admite una “explicación clásica”. Por otro lado, también depende de las medidas usadas en el experimento, ya que, por ejemplo, la implementación de observables que se puedan medir conjuntamente nunca puede dar lugar a violaciones de desigualdades de Bell. No existen muchos trabajos relacionados con el problema recíproco: si dos medidas que no se pueden medir conjuntamente pueden ser siempre usadas para conseguir una desigualdad de Bell.

El principal objetivo de este capítulo es dar caracterizaciones de medidas generalizadas (POVMs) que no son medibles simultáneamente. Una caracterización de estas medidas es bien conocida en el caso de medidas proyectivas, en términos de conmutatividad de las proyecciones asociadas a las medidas. Sin embargo, en el caso de medidas generalizadas no se conoce ningun criterio más allá de pares de medidas en qubits.

La herramienta principal que usamos en este trabajo es la identificación de una desigualdad del tipo CHSH con el dual lagrangiano de una expresión de la medibilidad conjunta, escrita como un problema de programación semidefinida. Esta relación nos permite establecer criterios simples para decidir si dos medidas generalizadas son simultáneamente realizables.

Como consecuencia, encontramos una novedosa relación entre dos importantes características de la teoría cuántica: la existencia de magnitudes que no se pueden medir conjuntamente y la no localidad cuántica. Además, esto nos permite concluir que dos medidas que no se pueden realizar simultáneamente en la Mecánica Cuántica tampoco podrán ser medidas conjuntamente en cualquier otra teoría no-signalling (que no permita comunicación superlumínica) que sea un refinamiento de la cuántica.

No localidad, desigualdades de Bell y teorías no-signalling. En el artículo que Einstein, Podolski y Rosen publicaron juntos en 1935, propusieron un experimento teórico que podría llevar a una posible incompletitud de la Mecánica Cuántica. Dado que dos partículas entrelazadas podrían "compartir" magnitudes conjugadas, uno podría ser capar de medir "simultáneamente" una de esas magnitudes en la primera de las partículas y la otra magnitud en la segunda. De este modo, se podría violar el Principio de Incertidumbre de Heisenberg. Concluyeron que debían de existir más "elementos de realidad" que determinaran esas magnitudes, que no estarían bajo nuestro control. Tales modelos han sido llamados modelos de variables ocultas (modelos LHV, de sus siglas en inglés).

La otra explicación posible sería admitir la no localidad de la naturaleza, asumiendo la existencia de "acciones a distancia". Al medir una de las partículas, la otra se vería automáticamente transformada por la acción realizada sobre la primera, y de tal modo la segunda magnitud ya no se podría medir con la precisión requerida. En tal caso se seguiría respetando el Principio de Incertidumbre, aunque esta alternativa parecía poco plausible: la posibilidad de estas acciones a distancia no fue inicialmente bien aceptada.

En 1964, Bell propuso un experimento sencillo que serviría para poder verificar la existencia de ese comportamiento no local de la naturaleza. El primer experimento en esa dirección fue realizado por Aspect en 1982 [**7**]. Existen aún, sn embargo, diversos problemas para poder verificar la existencia de esta no localidad de forma totalmente concluyente, debido principalmente a la eficiencia no óptima de los detectores de los experimentos, problema llamado *detection loophole* [**7, 98**].

Se pueden distinguir distintos tipos de distribuciones de probabilidad resultantes de experimentos. En primer lugar, están aquellas que pueden ser explicadas con modelos de variables ocultas; éstas forman un politopo, y son llamadas distribuciones de probabilidad clásicas o comportamientos clásicos, ya que pueden ser expresadas como combinaciones convexas de distribuciones explicables con teorías físicas clásicas. Un segundo conjunto, que incluye al anterior, es el de las distribuciones de probabilidad que pueden resultar de experimentos cuánticos; este conjunto ya no es un politopo, aunque sigue siendo convexo. Existen otros conjuntos cuyo estudio ha despertado interés (véase, por ejemplo, [**88**]), que dependen del tipo de propiedades físicas que se quieran asumir. Entre ellos, destaca el conjunto llamado *no-signalling*, también un politopo, en el que lo único que se asume es que la información no puede viajar a velocidad mayor que la de la luz.

Los hiperplanos que delimitan el conjunto de comportamientos clásicos da lugar a desigualdades corresponientes a los respectivos semiespacios en el que están las distribuciones clásicas. Estas desigualdades son llamadas desigualdades de Bell, y la diferencia entre los comportamientos clásicos y puramente cuánticos puede ser comprobada por la violación de una de estas desigualdades de Bell. Usamos un tipo concreto, ligeramente modificado, de estas desigualdades, que simplemente relaciona correlaciones de las distribuciones de probabilidad. El ejemplo más conocido es el de la desigualdad CHSH [**30**], que únicamente requiere dos medidas, cada una de las cuales puede tomar dos posibles valores ± 1.

El estudio de las desigualdades de Bell ha sido y sigue siendo una línea de investigación muy activa y fructífera, que ha llevado a multiples resultados, desde las cotas de Tsirelson [**122**] a la posibilidad de violaciones no acotadas de desigualdades de Bell tripartitas [**102**], entre muchos otros. También ha habido propuestas para usarlas como medida de entrelazamiento, y para innumerables aplicaciones. En esta línea, la rigidez de la desigualdad CHSH ha llevado a su uso en ciptografía cuántica independiente de la seguridad de los aparatos usados [**110**]. Además, la no localidad ha sido identificada como un recurso necesario para la distribución cuántica de claves [**12**], para la generación de aleatoriedad segura [**105**] o como recurso para el diseño de estrategias mejoradas en juegos cuánticos [**40, 81**].

Aunque el entrelazamiento del estado sobre el que se realiza la medida es necesario para que un experimento muestre no localidad, existen estados entrelazados que no violan ninguna desigualdad de Bell, y por tanto no pueden mostrar este comportamiento. En este capítulo nos preguntamos si la medibilidad conjunta de las medidas, que se sabe es una condición necesaria para la posibilidad de violación de una desigualdad de Bell, es también una condición suficiente. Mostramos que, dadas dos medidas no simultáneamente realizables, pueden ser siempre usadas para construir una desigualdad de Bell que, junto con algún estado, darían una violación de la misma y evidenciaría la existencia de distribuciones de probabilidad no locales.

Como consecuencia, relacionamos la medibilidad conjunta en la Mecánica Cuántica con la medibilidad conjunta en cualquier teoría no-signalling que sea compatible con la teoría cuántica.

Medidas conjuntas. El Principio de Incertidumbre de Heisenberg es otra de las consecuencias fundamentales de la Mecánica Cuántica. Este principio establece que existen magnitudes conjugadas que no pueden determinarse conjuntamente con exactitud: cuanto más precisa sea la medición de una de ellas, más imprecisa resultará la información que se obtenga de la otra. Esto es, en gran parte, consecuencia de que al efectuar una medida sobre un sistema éste se puede ver modificado, lo que no impide en algunos casos la medida secuencial de dos magnitudes.

El problema en el caso de medidas proyectivas simultáneamente realizables es bien conocido: dadas dos medidas proyectivas cuyos operadores de medida conmutan entre sí, existe otra medida proyectiva que permite recuperar los resultados de ambas, y por tanto permite efectuar ambas conjuntamente; por otro lado, si las proyecciones de las distintas medidas no conmutan entre sí, éstas no se pueden realizar conjuntamente.

Sin embargo, en el caso de medidas generalizadas sobre un sistema, llamadas POVMs (Positive Operator Valued Measurements), en las que no se tiene el control de todo el sistema sobre el que se realiza la proyección de la medida proyectiva, la equivalencia existente para medidas proyectivas deja de ser cierta. Dadas dos POVMs que conmuten, siempre se puede encontrar otra POVM que implemente ambas simultáneamente, pero también existen POVMs que no conmutan para las que tal tercera POVM se puede encontrar.

El objetivo de este capítulo es caracterizar la no medibilidad conjunta de las medidas generalizadas desde diferentes perspectivas: como un problema de mayoración entre operadores (semidefinidos) positivos, como un problema de optimización y, finalmente, mostrando que tales medidas pueden ser usadas para violar una desigualdad de Bell. El trabajo previo en relación con este problema concreto es escaso. No se conoce un criterio para la medibilidad conjunta de POVMs aparte del estudio realizado en [**24, 119, 137**] con sistemas de dos niveles, y la relación observada en [**4**] con la desigualdad CHSH para algunos observables particulares.

Existen más nociones relacionadas con la medibilidad conjunta que han sido estudiadas, como la coexistencia de efectos [**109**], la no perturbación [**61, 96**], la compatibilidad y la compatibilidad fuerte [**59**], etc., y otros problemas relacionados con el que nos planteamos, como la existencia de medidas conjuntas con información completa [**25**] y la aproximación simultánea de medidas incompatibles [**58**].

Programación semidefinida. La última herramienta que usamos para este problema es la programación semidefinida, aprovechando que la primera caracterización dada en términos de la existencia de un operador que respeta ciertas mayoraciones entre operadores positivos se puede reescribir como un problema de optimización en el lenguaje de programación semidefinida.

La programación semidefinida (SDP) es una clase de problemas de optimización convexa, que incluye, entre muchos otros, todos los problemas de programación lineal. Este tipo de problemas tiene como función objetivo una función lineal, pero el conjunto factible no está determinado por restricciones lineales, sino que está descrito con desigualdades en el retítulo de operadores hermíticos.

Los problemas SDP, bajo ciertas condiciones [**47**], están incluidos en la clase de problemas cuya solución se puede aproximar polinomialmente. Este tipo de problemas ha sido muy útil en el diseño de algoritmos para aproximar la solución de algunos problemas NP-hard clásicos, dando mejores aproximaciones que las anteriores aproximaciones obtenidas con programas lineales. En esta línea, la programación semidefinida ha dado buenos resultados en problemas de complejidad combinatoria, como algoritmos polinomiales exactos para colorear grafos perfectos, el cálculo de cotas tratables para la capacidad de Shannon de grafos, y las mejores aproximaciones conocidas para max-cut, particiones de grafos y minimización de discrepancias. En el campo de la información cuántica, la programación semidefinida ha sido aplicada a diversos problemas, llevando a interesantes resultados como, por ejemplo, aproximaciones del valor clásico de juegos XOR no locales (usando para ello también cotas de Tsirelson), y aproximaciones del valor cuántico de juegos no locales y problemas cuánticos en grafos (usando una jerarquía de relajaciones SDP).

Usaremos además el hecho de que el dual lagrangiano de un problema SDP también está en la clase SDP, y que si uno alcanza su óptimo el otro también lo hace, y estos valores coinciden. Este paso nos permitirá relacionar el problema de la medibilidad conjunta con la violación de desigualdades de Bell del tipo CHSH.

Resultados principales. En primer lugar, planteamos el problema de la medibilidad conjunta de dos observables dicotómicos (que pueden tomar únicamente dos valores). Cada uno de ellos puede ser descompuesto en dos operadores positivos, P y $\mathbb{I}-P$, y Q y $\mathbb{I}-Q$, respectivamente, llamados efectos. La primera caracterización que obtenemos, como un problema de mayoración entre operadores semidefinidos positivos, es la siguiente:

Proposición. *Dos observables, caracterizados respectivamente por dos efectos P y Q, son conjuntamente medibles si y sólo si existe un operador S semidefinido positivo tal que $Q+P-\mathbb{I}\leq S\leq P,Q$.*

Al menos un operador semidefinido positivo S tal que $S\leq P,Q$ siempre existe ($S=0$), lo que nos permite reescribir el resultado anterior como un problema de optimización, con un conjunto factible no vacío, calculando el valor del mínimo λ para el cual exista un operador semidefinido positivo S con $Q+P-\lambda\mathbb{I}\leq S\leq P,Q$:

Proposición. *Dos observables caracterizados por dos efectos P y Q son medibles conjuntamente si y sólo si la solución del problema de programación semidefinida*

$$\lambda_0=\text{ínf}\{\lambda\in\mathbb{R},\ Q+P\leq\lambda\mathbb{I}+S\},$$

con restricciones $0\leq S\leq Q,P$, es menor o igual a 1.

Tomando el dual y modificándolo ligeramente, obtenemos una nueva caracterización del problema en términos de la violación de una desigualdad del tipo CHSH para algún estado cuántico:

Teorema. *Dos observables, determinados por dos efectos P y Q respectivamente, no son conjuntamente medibles si y sólo si permiten la violación de una desigualdad de Bell. Cuantitativamente, existen dos observables POVM dicotómicos, que toman como valores ±1, tal que el supremo del operador CHSH*

$$\mathbb{B}=(A_1\otimes(B_1+B_2)+A_2\otimes(B_1-B_2))/2,$$

para $A_1=\mathbb{I}-2P$ y $A_2=2Q-\mathbb{I}$, sobre todos los posibles estados cuánticos es

$$\sup_\rho\left|\langle\mathbb{B}_\rho\rangle\right|=1+2\lambda_0^*,$$

mientras que $\left|\langle\mathbb{B}_\rho\rangle\right|\leq1$ para cualquier estado separable ρ.

También damos una caracterización computable de la medibilidad conjunta de dos POVMs dicotómicas:

Teorema. *El primer supremo del resultado anterior puede ser calculado con sólo hallar* $\lambda_0^* = \max_{\phi\in[0,\pi]} \mu(\phi)$ *donde* $\mu(\phi)$ *es el mayor autovalor de*

$$(Q + P - \mathbb{I}) \otimes \begin{pmatrix} c^2 & cs \\ cs & s^2 \end{pmatrix} - Q \oplus P,$$

para $c = \cos(\phi)$ *y* $s = \sin(\phi)$.

Finalmente, relacionamos los resultados previamente expuestos con el escenario no-signalling, dado que la violación de una desigualdad del tipo CHSH implica que los observables tampoco podrán ser medidos conjuntamente en cualquier otra teoría no-signalling compatible con la Mecánica Cuántica.

Además, discutimos brevemente los casos de varios observables dicotómicos, y los de observables que puedan tomar más de dos valores.

Hamiltonianos uncle para Matrix Product States.

Motivación. En sistemas multipartitos, el entrelazamiento se vuelve más complicado que en los sistemas bipartitos, dependiendo del número de partes en que se considere dividido el sistema. Siempre que se considere el espacio separado en más de dos regiones, no hay un modo natural de cuantificar este entrelazamiento, ni operaciones equivalentes a las que dan lugar al entrelazamiento de formación y al entrelazamiento destilable, debido a no haber estados máximamente entrelazados al aparecer tipos esencialmente distintos de entrelazamiento. Por ejemplo, en el caso tripartito, los estados W y GHZ,

$$|\mathrm{W}\rangle = \frac{|001\rangle + |010\rangle + |100\rangle}{\sqrt{3}}, \ |\mathrm{GHZ}\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}},$$

son un perfecto ejemplo de este hecho [**37**]. Sin embargo, cuando se considera el sistema dividido únicamente en dos partes, el estudio de la entropía de entrelazamiento tiene una gran utilidad en el contexto de sistemas con muchos cuerpos.

La mayor parte de los sistemas en equilibrio que aparecen en la naturaleza muestran una propiedad particular a temperatura cero: una ley de área para la entropía de entrelazamiento entre dos regiones disjuntas. Esto es, la entropía de entrelazamiento depende de la medida de la frontera que separa las dos regiones, en lugar de depender del tamaño de las dos regiones, como sucede para estados genéricos.

En sistemas unidimensionales, los Matrix Product States (MPSs), inicialmente conocidos como estados finitamente correlados, es una familia de estados muy adecuada para atacar problemas en este contexto. Estos estados capturan en gran medida la física de las interacciones locales en sistemas de una dimensión.

Desde el punto de vista del análisis numérico, los MPSs son el conjunto variacional de toda una serie de algoritmos basados en métodos de renormalización. La descripción de los MPSs es muy eficiente, lo que ayuda a evitar el problema de tener que controlar un número exponencial de parámetros para describir los estados. Existen diversos resultados teóricos que garantizan la capacidad de los MPSs para aproximar estados "naturales", tales como los resultados de Hastings relacionando estados fundamentales de hamiltonianos con gap con la ley de área y el decaimiento exponencial de correlaciones, y el trabajo de Brandao y Horodecki relacionando este decaimiento de correlaciones con los MPSs.

Los Matrix Product States también han sido útiles en el problema de clasificación de fases de la materia en una dimensión, y en aclarar el papel de las simetrías y su relación con los llamados *string order parameters*. Para conseguir tales resultados, ha sido crucial el hecho de que a cada MPS se le puede hacer corresponder de forma natural un hamiltoniano, el hamiltoniano *parent*, que tiene al MPS como estado fundamental. Los hamiltonianos, que codifical las interacciones presentes en los sistemas, determinan la evolución de los mismos. A temperatura cero los sistemas se estabilizan en sus estados fundamentales, que son los autoestados asociados a los mínimos autovalores de los respectivos hamiltonianos, y son sobre los que se puede intentar medir propiedades físicas de los sistemas.

Dado un hamiltoniano, sus estados fundamentales están determinados. Sin embargo, dado un estado hay distintos hamiltonianos para los cuales el estado es un estado fundamental. Este hecho, motiva las siguientes preguntas: ¿cuán robusto es la construcción del hamiltoniano parent asociado a un MPS dado? Y, ¿pueden existir otros hamiltonianos que tengan al mismo MPS como estado fundamental pero que muestre propiedades distintas de las que tiene el hamiltoniano parent?

Éste es el objetivo del trabajo que presentamos en este capítulo. Consideramos los hamiltonianos parent correspondentes a pequeñas perturbaciones de un MPS dado, y tomamos el límite cuando hacemos la perturbación desaparecer. Cuando este límite es diferente del hamiltoniano parent del MPS original, lo que puede suceder sólo si el MPS es no inyectivo, el nuevo hamiltoniano límite es llamado el hamiltoniano *uncle*, cuyas propiedades (espacio de estados fundamentales y espectro) estudiamos. Como resultado, encontramos que el hamiltoniano uncle y el hamiltoniano parent tienen los mismos estados fundamentales, pero que difieren en sus propiedades espectrales: el hamiltoniano uncle no presenta gap espectral, mientras que el hamiltoniano parent sí tiene gap. Tanto el estudio de los estados fundamentales como del espectro se hace en el caso de cadenas finitas e infinitas (en el límite termodinámico). Además, para MPSs inyectivos, para los que la construcción del hamiltoniano parent es robusta, consideramos una descripción no inyectiva de los mismos para construir hamiltonianos uncle para ellos. En este caso los resultados obtenidos son similares, excepto en el estudio del espacio de estados fundamentales para cadenas finitas, ya que para el hamiltoniano uncle este espacio es mayor que para el hamiltoniano parent.

Matrix Product States. La descripción de un estado genérico de un sistema compuesto de un número n grande de partículas es muy compleja. Si cada partícula puede ser descrita con un espacio de Hilbert de dimensión d, el sistema compuesto tendrá asociado un espacio de dimensión d^n. Por tanto, se necesitaría controlar un número exponencialmente grande de parámetros a la hora de realizar cualquier tipo de cálculo.

Sin embargo, las interacciones de la naturaleza son altamente locales, por lo que aquellos estados que efectivamente aparecen como estados fundamentales de hamiltonianos determinados por estas interacciones son únicamente una pequeña porción del conjunto de todos los estados. Para sistemas en retículos unidimensionales, esta propiedad parece ser bien descrita por los llamados Matrix Product States, que son unos estados cuyos coeficientes pueden describirse como productos de ciertos conjuntos de matrices $\{A_i^{[k]},\ i = 1,\dots,d,\ k = 1,\dots,n\}$ de la forma

$$|\varphi\rangle = \sum_{i_j=1}^{d} \operatorname{tr}(XA_{i_1}^{[1]}A_{i_2}^{[2]}\cdots A_{i_3}^{[3]})|i_1 i_2 \dots i_n\rangle \ ,$$

donde X determina las condiciones de contorno, puras ($X = |r\rangle\langle l|$) o mixtas.

De hecho, cualquier estado admite una descripción como Matrix Product State si la dimensión de las matrices es suficientemente grande, lo que puede ser probado tomando descomposiciones de Schmidt sucesivas del estado y guardando los coeficientes resultantes adecuadamente en las matrices. A pesar de ello, trabajar con tales descripciones podría llegar a ser incluso más costoso que hacerlo directamente con los coeficientes del estado respecto a alguna base. La gran utilidad de los MPSs surge del hecho de que, para los estados "naturales" mencionados previamente, estos MPSs permiten una aproximación eficiente de los mismos.

La localidad de las interacciones que determinan la evolución de los sistemas, hace que los estados cuánticos físicamente relevantes presenten algunas propiedades especiales: estos estados usualmente muestran un rápido decaimiento con la distancia de las correlaciones entre dos partículas y una propiedad llamada ley de área para la entropía de entrelazamiento, esto es, dada una separación del sistema en dos regiones, la entropía de entrelazamiento depende del tamaño de la frontera separando las dos regiones en lugar de depender del tamaño de las regiones. Los MPSs satisfacen esta ley de área, ya que la entropía de entrelazamiento está acotada por la dimensión de las matrices adyacentes al corte hecho para la separación del sistema en dos regiones.

La relación entre estados fundamentales de hamiltonianos determinados por interacciones locales (llamados hamiltonianos locales), esta ley de área y la tasa de decaimiento de las correlaciones en estos estados ha sido objeto de diversos trabajos. En [**57**] Hastings probó que los estados fundamentales de hamiltonianos locales con gap[2] presentan un decaimiento exponencial de correlaciones, y Brandao y Horodecki mostraron en [**19**] que los estados de sistemas unidimensionales que muestran tales correlaciones pueden ser bien aproximados por MPSs, mejorando un resultado previo de Hastings [**56**] en el que se requería que el estado fuera además un estado fundamental de un hamiltoniano local con gap. Existen otros resultados recientes en esta línea, como [**6**], en el que se mejoran exponencialmente los parámetros de [**56**], o [**72**], en el que los autores dan un algoritmo probabilístico polinomial para aproximar estados fundamentales de hamiltonianos locales

[2]Más adelante, describiremos distintas nociones de gap espectral. En estos resultados la noción usada es la más fuerte de ellas, que supone unicidad del estado fundamental.

con gap en una dimensión.

Todos estos resultados van más allá de sus implicaciones teóricas, ya que dan soporte a la gran efectividad de metodos numéricos basados en técnicas de renormalizacion, para los que los MPSs son una herramienta esencial [**92, 111, 129**].

Además, los MPSs no sólo sirven para aproximar eficientemente estados fundamentales de sistemas unidimensionales, sino que también describen de forma exacta una gran familia de estados interesantes, como pueden ser los estados GHZ [**49**], los estados W [**37**], los estados *cluster* en una dimensión [**22**], los estados AKLT [**1**], etc., usando para ello matrices de dimensión baja. Los MPSs también se pueden usar para describir estados generados secuencialmente [**113**], y para ciertas tareas en computación cuántica basada en medidas [**50**].

Entre otros resultados teóricos, el papel de los MPSs en la descripción de la física de sistemas unidimensionales ha facilitado la compresión del papel de las simetrías en cadenas de *spins* [**114**] y ha permitido la clasificación de las fases cuánticas con gap en sistemas unidimensionales [**27, 42, 107, 115**].

La estructura de los MPSs se puede extender a retículos de otras dimensiones, a los llamados Projected Entangled Pair States (PEPSs, [**126**]). Aunque para PEPSs no existen aún resultados tan fuertes como existen para MPSs apoyando su papel en el problema de aproximar estados fundamentales de hamiltonianos locales (podríamos destacar [**55**] entre los resultados obtenidos), también son una muy buena herramienta para el diseño de métodos numéricos [**95**] y han llevado a diversos resultados teóricos y aplicaciones prácticas, en parte gracias a la relación entre algunas de sus propiedades y el retículo sobre el que están definidos. También trabajamos, en otro capítulo, con el caso de PEPSs en retículos de dimensión dos, principalmente con uno de los ejemplos paradigmáticos, el código tórico de Kitaev [**67**].

Hamiltonianos asociados. Como acabamos de comentar, los MPSs aproximan eficientemente los estados fundamentales de hamiltonianos locales con gap[3] y describen exactamente muchos estados interesantes usando matrices de dimensión baja.

En el sentido contrario, cualquier MPS es un estado fundamental de algún hamiltoniano local. Uno de esos hamiltonianos, que se puede asociar de forma natural a cualquier MPS, es el llamado hamiltoniano parent [**41, 101**], cuyas interacciones locales están representadas por proyecciones. Bajo una condición bastante general, llamada inyectividad del MPS, el hamiltoniano parent presenta gap espectral y tiene al correspondiente MPS como único estado fundamental. Además, para MPSs traslacionalmente invariantes, la forma normal encontrada en [**101**] determina claramente la dimensión del espacio de estados fundamentales, dependiendo de su inyectividad o inyectividad por bloques. Los hamiltonianos parent son una de las herramientas principales que usamos en los resultados de este capítulo.

[3] De nuevo, noción fuerte de gap.

Los hamiltonianos parent están determinados por la descripción matricial de los MPSs, correspondiendo por tanto a una asignación[4] de conjuntos de matrices a hamiltonianos locales,

$$A \mapsto \hat{H}(A)\ .$$

El principal objetivo de este capítulo es estudiar la robustez de esta construcción. Esto es, ¿llevan perturbaciones lineales continuas $A + \varepsilon P$ de las descripciones matriciales a transformaciones continuas de los hamiltonianos parent asociados? La respuesta no siempre es positiva, como ya se observó en [**26**] para retículos de dos dimensiones.

En aquellos casos en que la respuesta a la pregunta es negativa, consideramos los hamiltonianos límite

$$H'_P(A) = \lim_{\varepsilon \to 0} \hat{H}(A + \varepsilon P),$$

a los que llamamos hamiltonianos *uncle*, para los que el MPS descrito por el conjunto de matrices A es también un estado fundamental. También estudiamos todo su espacio de estados fundamentales, comparándolo con el correspondiente al hamiltoniano parent de partida.

Debemos señalar que las perturbaciones inducidas en los hamiltonianos por este procedimiento no son en general pequeñas, por lo que los resultados que presentamos no entran en contradicción con trabajos como [**80**] sobre la estabilidad de hamiltonianos locales bajo pequeñas perturbaciones de los mismos.

Gap espectral y límite termodinámico. Otro concepto fundamental de los hamiltonianos sobre retículos es el de gap espectral. Se dice que una familia de hamiltonianos, definida sobre sistemas en retículos finitos de tamaño creciente, tiene gap si existe una cota uniforme $\Delta > 0$, independiente del tamaño del retículo, entre el menor autovalor de cada hamiltoniano y el resto de autovalores del mismo. Existen otras nociones de gap, dependiendo del problema a tratar. Una versión más fuerte es considerar que aquellos hamiltonianos cuyo espacio de estados fundamentales tiene dimensión mayor que uno nunca puede tener gap, en cuyo caso se dice que este espacio es degenerado. Por otro lado, una relajación de la primera definición dada es requerir la existencia de una cota uniforme entre unos cuantos autovalores mínimos distintos y el resto de autovalores del hamiltoniano, y que esos autovalores mínimos tiendan al mismo valor cuando el tamaño del retículo crezca, lo que recibe el nombre de *ground space splitting*.

En relación con el estudio de los espectros para cadenas crecientes, también se pueden estudiar las propiedades de los hamiltonianos en cadenas infinitas, lo que recibe el nombre de límite termodinámico. Su formalización requiere algunas herramientas adicionales, tales como considerar la imagen de Heisenberg de las evoluciones y manejar operadores no acotados y representaciones GNS de las álgebras de observables. En esta imagen dual, se considera que la evolución unitaria determinada por el hamiltoniano actua sobre los observables en lugar de sobre los estados, y los estados son funcionales sobre los observables dando como resultado el valor esperado de la medida de los mismos. Éste es el punto de vista de los estados en el contexto de C^*-álgebras. Se dice que un hamiltoniano en el límite termodinámico tiene gap si su menor valor espectral está aislado en el espectro. También ahora puede haber diferentes definiciones de gap, dependiendo de si se requiere

[4]Una vez fijado el rango de las interacciones locales.

que el espacio de estados fundamentales tenga dimensión igual a uno o no.

La noción de gap es crucial en el problema de clasificación de fases de la materia. Se dice que dos estados están en la misma fase si existe un camino continuo de hamiltonianos con gap H_s tales que esos dos estados son estados fundamentales de H_0 y H_1 respectivamente y, además, el gap no se cierra a lo largo del camino: $\Delta_s > 0$. La existencia de gap espectral es también importante para la estabilidad de los estados fundamentales ante imperfecciones físicas [**80**] y para poder aplicar algoritmos eficientes para encontrar estos estados fundamentales [**72**].

A la hora de estudiar el gap de hamiltonianos en cadenas finitas e infinitas se ha de tener cuidado con los posibles efectos existentes en los bordes de cadenas finitas abiertas, pues éstos pueden desaparecer en el límite termodinámico [**13, 41**].

En relación con nuestro problema, los hamiltonianos parent muestran gap espectral sobre el mínimo nivel de energía [**41**] (sea el autoespacio degenerado o no). Estudiamos esta propiedad en los hamiltonianos uncle, probando que éstos no presentan ese gap espectral.

Resultados principales. Como ya se ha mencionado, los principales objetivos de este capítulo son el estudio de la robustez del hamiltoniano parent y de la relación entre estados fundamentales y hamiltonianos. En primer lugar, mostramos que dado un MPS inyectivo, la perturbación de su descripción tensorial induce perturbaciones continuas del hamiltoniano parent. Por tanto, centramos nuestro estudio en el caso de MPSs inyectivos por bloques. En este caso, lo mismo sucede cuando la perturbación respeta la estructura de bloques del MPS. Cuando la perturbación inducida no es continua construimos el llamado hamiltoniano uncle. Detallamos los resultados para el caso de MPSs de dos bloques, pero los resultados pueden extenderse con toda generalidad a MPSs de más bloques.

La primera propiedad que estudiamos es el espacio de estados fundamentales de los hamiltonianos uncle para cadenas cerradas, es decir, con condiciones de contorno periódicas ($X = \mathbb{I}$). Esto nos lleva al primer resultado:

> TEOREMA. *Dado un un MPS con condiciones de contorno periódicas descrito por un tensor A inyectivo por bloques, para casi toda perturbación*[5] *P el espacio de estados fundamentales del hamiltoniano uncle H'_P coincide con el espacio de estados fundamentales del hamiltoniano parent.*

Además, damos condiciones fácilmente verificables sobre la perturbación P para que el hamiltoniano uncle cumpla este resultado.

La segunda propiedad que estudiamos es el gap espectral de los hamiltonianos uncle sobre cadenas finitas, llegando a este segundo resultado:

[5]En éste y en los siguientes resultados, casi toda perturbación quiere decir salvo a lo sumo una variedad algebraica.

TEOREMA. *Dado un un MPS con condiciones de contorno periódicas descrito por un tensor A inyectivo por bloques, para casi toda perturbación P el hamiltoniano uncle no presenta gap.*

Este hecho contrasta con la presencia de gap en los hamiltonianos parent. Cuando consideramos cadenas infinitas obtenemos resultados similares en el límite termodinámico.

TEOREMA. *Dado un un MPS descrito por un tensor A inyectivo por bloques, para casi toda perturbación P el hamiltoniano uncle H'_P tiene el mismo espacio de estados fundamentales en el límite termodinámico que el hamiltoniano parent. Además, el hamiltoniano uncle no presenta gap espectral para casi toda perturbación P, y su espectro es toda la semirrecta real positiva.*

Dado el papel que tiene el gap espectral en la clasificación de fases, estos resultados apuntan a que hay que tener cierta precaución cuando se intente definir esta clasificación en el nivel de los estados en lugar de en el nivel de las interacciones que determinan los hamiltonianos, ya que el mismo estado puede ser estado fundamental de hamiltonianos con propiedades espectrales distintas, aún compartiendo todo el espacio de estados fundamentales.

Finalmente, el estudio del límite termodinámico de los hamiltonianos uncle nos permite obtener información adicional de los espectros para cadenas finitas.

TEOREMA. *Dado un un MPS con condiciones de contorno periódicas descrito por un tensor A inyectivo por bloques, para casi toda perturbación P los espectros del hamiltoniano uncle H'_P sobre cadenas finitas de tamaño creciente tienden a ser densos en la semirrecta real positiva.*

Aunque en el caso de MPSs inyectivos la perturbación inducida en los hamiltonianos parent es continua, usando una descripción no inyectiva de los mismos podemos construir también hamiltonianos uncle para estos estados. En este caso, los resultados espectrales obtenidos para MPSs no inyectivos siguen siendo válidos. La única diferencia en este nuevo caso es que el espacio de estados fundamentales del hamiltoniano uncle para cadenas finitas ya no coincide con el del hamiltoniano parent. En el límite termodinámico estos espacios sí coinciden, teniendo al MPS como único ground state.

Hamiltoniano uncle para el código tórico.

Motivación. La generalización de los Matrix Product States a retículos de más dimensiones son los llamados Projected Entangles Pair States (PEPSs), cuyo nombre proviene de uno de los procedimientos para construirlos, proyectando[6] estados máximamente entrelazados dispuestos en las aristas del retículo, con una aplicación determinada por un tensor. En el caso unidimensional este tensor puede ser visto como un conjunto de matrices, de donde viene el nombre Matrix Product States; en el caso de retículos de dimension dos los tensores tendrán cinco índices, lo que corresponde a conjuntos de tensores de cuatro índices.

Los PEPSs comparten muchas propiedades con los MPSs: satisfacen la ley de área para la entropía de entrelazamiento, son estados fundamentales de hamiltonianos parent [**100**], tienen métodos eficientes para calcular de forma aproximada valores esperados, dan descripciones exactas de cualquier estado para tensores suficientemente grandes, describen muchos estados interesantes con tensores de dimensión baja, pueden ser usados para computación cuántica basada en medidas (en este caso universal) [**130**], etc. Por el contrario, no existe una forma normal para ellos, la inyectividad del tensor no implica que el hamiltoniano parent tenga gap [**100**], y no se ha demostrado aún que aproximen eficientemente los estados fundamentales de hamiltonianos locales con gap. A pesar de ello, son una muy buena herramienta para el diseño de métodos numéricos, como se ha visto en numerosos trabajos [**95**]. Y, dejando a un lado las aplicaciones numéricas, los PEPSs son muy útiles para intentar entender una propiedad que muestran algunos sistemas en dos o más dimensiones [**114**]: el orden topológico.

El estudio de fases con orden topológico en la Física de la Materia Condensada comenzó en los años 80, con el descubrimiento del efecto Hall cuántico fraccionario y la superconductividad a altas temperaturas. En el campo de la información cuántica, el interés por este tipo de fases creció cuando Kitaev mostró el que desde entonces es uno de los ejemplos paradigmáticos de orden topológico: el código tórico. Las propiedades de esta familia de estados hace que algunos de ellos puedan ser usados en diversas aplicaciones, tales como computación cuántica universal más robusta o su uso como memoria cuántica estable.

En este capítulo, como en el anterior, nos interesamos por el problema de la relación entre estados fundamentales y hamiltonianos. Trabajamos con el código tórico, usando su descripción como PEPS, y su hamiltoniano parent asociado para obtener un nuevo hamiltoniano sin gap, el hamiltoniano uncle para el código tórico, que tiene al código como espacio de estados fundamentales.

Orden topológico y el código tórico. En [**67**], Kitaev propuso un hamiltoniano local y su espacio de estados fundamentales, el código tórico, cuyas propiedades han llevado a todo un nuevo paradigma desde el punto de vista de la información cuántica: la computación cuántica topológica. En el mismo artículo, propuso también las primeras generalizaciones del código tórico, los llamados modelos *quantum double*. Desde entonces,

[6]Aunque la aplicación que se efectúa recibe el nombre de proyección, no lo es en general.

ha habido muchos avances en este sentido.

Kitaev propuso el espacio de estados fundamentales de ese hamiltoniano local y sus excitaciones de baja energía como un modelo donde poder hacer computación cuántica resistente a errores. Aunque se mostró más tarde que su modelo mostraba algunas debilidades, las propiedades que tiene se han extendido a otros modelos más robustos que pueden ser usados como memorias cuánticas [**2, 21, 33, 51**] y para realizar computación cuántica [**89**]. La información es guardada en las excitaciones de baja energía o *anyons*, que pueden ser vistos como cuasipartículas, y las puertas lógicas se pueden implementar simplemente "trenzándolas". Estas cuasipartículas muestran estadísticas de trenzado más allá de los tipos bosónicos y fermiónicos usuales.

Algunas de las propiedades que muestran estos estados dependen de la topología del sistema, como por ejemplo la degeneración del espacio de estados fundamentales, y otras son también intrínsecamente topológicas, como las estadísticas de trenzado de las excitaciones, lo que da lugar al nombre orden topológico. Esta propiedad genérica se completa con otras características, como pueden ser la indistinguibilidad local de los estados fundamentales, correcciones topólogicas a la ley de área para la entropía de entrelazamiento [**68**], y hamiltonianos con gap estable ante perturbaciones locales.

Se puede ver que algunas de estas propiedades dependen únicamente de los estados, mientras que otras dependen del hamiltoniano para el que son estados fundamentales, y la relación entre todas estas propiedades aún no es del todo clara. Por tanto, la pregunta de si un mismo estado o familia de estados puede formar el espacio de estados fundamentales de distintos hamiltonianos con propiedades espectrales diferentes (hablando principalmente de gap) es importante en este contexto.

La mayor parte de los sistemas topológicos conocidos tienen una descripción en términos de PEPSs, como se ve en [**114**]. En este trabajo, los autores estudian el papel de las simetrías locales en estos comportamientos topológicos. PEPSs con tales simetrías, dando lugar a algunos de estos modelos topológicos, son los llamados PEPSs G-isométricos. En el caso del código tórico, éste puede ser descrito como un PEPS $\mathbb{Z}_2$-isométrico.

Partiendo de la falta de robustez de la construcción del hamiltoniano parent, mostrada por primera vez en [**26**], extendemos las técnicas del capítulo anterior a retículos de dimensión dos para estudiar nuevos hamiltonianos para modelos topológicos. Usamos para ello el código tórico, con su descripción en términos de PEPSs, para construir un hamiltoniano uncle para el código tórico. La ausencia de una forma normal para PEPSs no nos permite estudiar el problema con toda generalidad, como en el caso de MPSs, aunque los resultados pueden extenderse a otros estados topológicos, como por ejemplo los *Resonating Valence Bond States*, que también tienen una descripción como PEPS con cierta simetría $\mathbb{Z}_2$ [**116**].

Resultados principales. Partiendo de la descripción del código tórico en términos de PEPSs y del hamiltoniano parent asociado, tomamamos una perturbación del mismo inducida por una perturbación particular del tensor PEPS. Tomamos ésta en la dirección ortogonal a la proyección del PEPS, y tomamos el límite de los hamiltonianos parent cuando esta perturbación se desvanece, dando lugar al hamiltoniano uncle. Este nuevo hamiltoniano es distinto del hamiltoniano parent original, como se puede ver en las interacciones locales que los definen, y muestra similitudes y diferencias interesantes con el hamiltoniano parent del que proviene.

En primer lugar, estudiamos el espacio de estados fundamentales del nuevo hamiltoniano para condiciones de contorno periódicas, llegando al primer resultado:

> TEOREMA. *El hamiltoniano parent y el hamiltoniano uncle del código tórico tienen el mismo espacio de estados fundamentales para condiciones de contorno periódicas.*

En segundo lugar, estudiamos el espectro del hamiltoniano uncle. El hamiltoniano parent presenta gap espectral, ya que sus términos locales conmutan entre sí. En cambio, el nuevo hamiltoniano tiene diferentes propiedades:

> TEOREMA. *El hamiltoniano uncle para el código tórico en retículos finitos de tamaño creciente con condiciones de contorno periódicas no presenta gap espectral.*

Estas dos propiedades siguen siendo ciertas en el límite termodinámico, tanto si consideramos una de las dimensiones del retículo fijas como si permitimos ambas tender a infinito.

> TEOREMA. *El hamiltoniano uncle y el hamiltoniano parent para el código tórico tienen el mismo espacio de estados fundamentales en el límite termodinámico. Por el contrario, mientras que el hamiltoniano parent tiene gap, el hamiltoniano uncle no lo tiene, y su espectro es toda la semirrecta real positiva.*

Como resultado final, y gracias al estudio del límite termodinámico del hamiltoniano uncle, somos capaces de obtener más propiedades espectrales de este hamiltoniano en retículos finitos.

> TEOREMA. *Los espectros del hamiltoniano uncle para el código tórico en retículos finitos con condiciones de contorno periódicas tienden a ser densos en la semirrecta real positiva.*

Conclusiones y trabajo futuro.

La mayor parte de las conclusiones han sido ya mencionadas en la exposición del trabajo realizado. Las recogemos de nuevo en esta sección, junto con preguntas y problemas sobre los que sería interesante trabajar en el futuro.

Espacios invariantes por reordenamiento en productos tensoriales. En lo que respecta al problema de la convertibilidad de estados, hemos encontrado que la estructura de invariancia por reordenamiento y la multiplicatividad de los problemas considerados son lo únicos elementos necesarios para caracterizar este problema en los escenarios ELOCC y MLOCC. Además, desde el punto de vista de la utilidad de los resultados en el campo de las Matemáticas, hemos encontrado una caracterización de los espacios ℓ_p y c_0 entre los espacios con base simétrica. También hemos extendido el problema a espacios invariantes por reordenamiento sobre espacios de medida continuos, obteniendo una caracterización para los espacios L_p en términos de propiedades multiplicativas.

Como consecuencia se puede deducir que no puede existir un teorema similar al de Pisier-Schütt en bases simétricas, ya que hemos expuesto dos ejemplos que contradirían tal resultado. Sin embargo, cabría plantearse el problema con condiciones más fuertes sobre la norma: ¿podría existir un teorema similar al de Pisier-Schütt para bases simétricas si nos restringimos a normas tensoriales? En tal caso, los resultados que hemos obtenido indican que las únicas posibilidades serían los espacios ℓ_1 y c_0, con las normas proyectiva e inyectiva respectivamente.

El trabajo de este capítulo, junto con otro posterior probando los mismos resultados [**11**], ha motivado un trabajo de Leinster sobre una caracterización multiplicativa de las medias de potencias (*power means*), que son los análogos no necesariamente positivos de las normas p, del tipo $\sum_{i=1}^{n} x_i^p$, donde puede haber además diferentes pesos para cada una de las coordenadas.

Finalmente, volviendo al contexto cuántico, sería interesante estudiar el problema de convertibilidad en el caso tripartito. ¿Puede ser considerada algún tipo de estructura simétrica relacionada con la caracterización LU ya existente, y puede esta estructura llevar a cierto orden que caracterice de manera sencilla la convertibilidad LOCC?

Medidas conjuntas y desigualdades de Bell. En el problema de la medibilidad conjunta de medidas generalizadas, hemos encontrado una novedosa relación entre dos de las más importantes consecuencias de la Mecánica Cuántica: el Principio de Intertidumbre y la no localidad de la naturaleza. El resultado no es sólo cualitativo sino también cuantitativo, ya que la máxima violación que se puede obtener usando dos medidas dicotómicas para una desigualdad del tipo CHSH está directamente relacionada con el grado de incertidumbre que es necesario introducir en las medidas para que éstas sean simultáneamente realizables. También hemos obtendo una condición fácilmente calculable para decidir si dos medidas dicotómicas generalizadas se pueden realizar conjuntamente o no.

Sin embargo, no hemos sido capaces de establecer una relación clara entre nuestros resultados y los trabajos previos existentes para qubits. Aunque conseguir tal relación no supondría ningún avance, su estudio podría llevar a extender la misma para poder conseguir caracterizaciones algebraicas, a partir de nuestros resultados, más allá de qubits.

Más relaciones entre los distintos tipos de medibilidad conjunta y entre la incertidumbre y la no localidad han sido encontradas posteriormente. Por ejemplo, se ha demostrado que la coexistencia no implica medibilidad conjunta [**109**], o se ha estudiado la posibilidad de *steering* óptimo [**94**].

También hemos obtenido ciertas caracterizaciones de la mediblidad conjunta para más de dos observables dicotómicos, y para dos observables que puedan tomar más de dos valores. Para estos casos una reducción similar a una desigualdad del tipo CHSH no es siempre posible, pues considerando únicamente incompatibilidades dos a dos, o agrupando resultados de medidas, no se consigue describir el problema completo.

Hamiltonianos uncle para Matrix Product States. En esta parte hemos estudiado el problema de la robustez del hamiltoniano parent para Matrix Product States casi en toda generalidad. Hemos construido hamiltonianos uncle tanto para MPSs no inyectivos como para MPSs inyectivos, y estudiado su espacio de estados fundamentales y propiedades espectrales: mientras que los hamiltonianos parent presentan gap espectral, los hamiltonianos uncle no lo presentan y su espectro tiende a ser denso en la semirrecta real positiva, y los espacios de estados fundamentales coinciden para los hamiltonianos parent y los hamiltonianos uncle en el caso de MPSs inyectivos por bloques.

La principal consecuencia de estos resultados se basa en el papel que tiene el gap espectral para la clasificación de fases de la materia: dependiendo de cómo se clasifiquen estas fases y del camino de hamiltonianos que se considere se puede encontrar a un estado bien en una fase o bien en una transición de fase. Aunque ya existían algunos ejemplos de estados asociados a distintos hamiltonianos con propiedades espectrales distintas, en este trabajo construimos sistemáticamente hamiltonianos con estas propiedades para MPSs, conectándolos con la falta de robustez del hamiltoniano parent. Finalmente, los hamiltonianos uncle pueden servir de herramienta para clasificaciones de estados más finas, en la línea de otros trabajos como [**13**].

Los hamiltonianos uncle no evidencian ningún posible problema en la aplicación de métodos numéricos basados en MPSs, ya que éstos parten de un hamiltoniano fijo que no varía durante el proceso de minimización de energía usado. Sin embargo, para el problema contrario de, dado un estado, encontrar las interacciones que lo hacen aparecer como estado fundamental usando métodos tomográficos, los hamiltonianos uncle muestran que la respuesta puede no ser única si se aplican métodos basados en MPSs.

Tan sólo hemos considerado perturbaciones lineales. Para el caso de perturbaciones no lineales, se pueden obtener los mismos resultados cuando el término dominante es la aproximación lineal de las mismas. Cuando éste no es el caso, tan sólo es necesario recurrir a aproximaciones de mayor grado para construir el tensor que determina el hamiltoniano uncle.

Una cuestión relacionada que merecería atención es el hecho de que, bajo perturbaciones del tensor, se puede detectar una discontinuidad en la entropía de entrelazamiento. De hecho, éste fue el primer efecto observado en relación con la falta de robustez del hamiltoniano parent en dos dimensiones [**26**], y se puede comprobar fácilmente que también sucede para la descripción de los estados GHZ como MPSs. Esta característica podría dar un nuevo punto de vista del problema desde el punto de vista de los estados, en lugar del punto de vista de los hamiltonianos que hemos tomado en nuestro trabajo.

Otro trabajo relacionado en el que estamos interesados es [**52**], en el que se considera una propuesta de algoritmo variacional para el cálculo de excitaciones basado en el formalismo de MPSs, y que está íntimamente relacionado con las excitaciones que usamos para demostrar que el hamiltonano uncle no tene gap. Este punto de vista encaja dentro del marco desarrollado en varios trabajos en que se ve al conjunto de MPSs como una variedad, considerando estas excitaciones como elementos del espacio tangente o estudiando la geometría de esta variedad y sus aplicaciones a métodos numéricos [**53**].

Hamiltoniano uncle para el código tórico. En el caso de retículos de dimensión dos y Projected Entangled Pair States, el problema de determinar qué perturbaciones inducen cambios continuos en el hamiltoniano parent está lejos de ser resuelta. Damos un ejemplo de perturbación sin esta propiedad, que puede ser generalizado a otras perturbaciones del mismo PEPS y a otros PEPSs (PEPS G-inyectivos), en los que la pregunta de la estabilidad se puede contestar fácilmente en términos de las simetrías del tensor y de la perturbación [**26**]. La pregunta general de qué tipo de perturbaciones tensoriales son físicas parece, sin embargo, mucho más complicada y un buen problema a tratar. En esta dirección, en [**29**] se puede ver una candidata a definición de qué perturbaciones deben ser consideradas naturales, aunque esta definición no permite decidir fácilmente cuáles lo son y cuáles no.

El hamiltoniano uncle que hemos construido para el código tórico es un ejemplo sencillo de un hamiltoniano sin gap para un sistema con orden topólogico, característica usualmente asociada a hamiltonianos con gap. Esta construcción tiene por tanto implicaciones en el estudio de clasificación de fases de la materia, debido al papel que el gap espectral tiene en él, y da argumentos a favor de la necesidad de considerar esta clasificación involucrando tanto el nivel de los estados como el nivel de los hamiltonianos.

Como hemos comentado, se pueden dar fácilmente otros hamiltonianos uncle para PEPSs G-inyectivos. En el caso de PEPS $\mathbb{Z}_2$-inyectivos, entre los que están los Resonating Valence Bond States [**116**], tendríamos una construcción muy similar. El hamiltoniano uncle tendría el mismo espacio de estados fundamentales que el hamiltoniano parent y no tendría gap. Sin embargo, no está claro que se pudiera garantizar que el espectro es toda la semirrecta real positiva cuando la dimensión del retículo crece. Para probar este hecho para el código tórico, nos hemos apoyado en la estructura $\mathbb{Z}_2$-isométrica del PEPS, y en el caso previo de MPSs en la existencia de una forma normal, que ya no tenemos en este caso. Para PEPSs G-isométricos (y G-inyectivos) habría que prestar especial atención al problema de determinar el espacio de estados fundamentales cuando se cierran las condiciones de contorno al probar la llamada propiedad de intersección (Prop. 6.4.2), que no ha supuesto una gran dificultad en nuestro trabajo gracias a que el grupo de simetría era $\mathbb{Z}_2$; en este sentido, debemos observar que la prueba de esta propiedad para hamiltonianos parent en el caso de PEPS G-inyectivos dada en [**114**] está lejos de ser trivial.

Otro problema que hemos empezado a considerar es el del papel de simetrías locales y globales en diferentes niveles de los PEPSs. Si uno toma varias copias de un PEPS G-inyectivo, y considera la imagen bajo cierta aplicación simetrizante, uno obtiene un nuevo PEPS con una simetría G en cada copia y una simetría global entre las distintas copias. Esto puede dar lugar a nuevos modelos topológicos interesantes, debido a la aparición de diferentes excitaciones aniónicas[7] resultantes de combinar las excitaciones de los diferentes niveles [**97**].

[7]Relacionadas con las cuasipartículas anyons, no con aniones (anions) en el sentido usual.

Mathematical methods for problems on entanglement: state convertibility, joint measurability, and Hamiltonians on PEPS

by

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CHAPTER 1

Introduction.

The interest of mankind towards description and prediction of natural phenomena has been a constant in Science. One of the most recent theories we can count with now is Quantum Theory, which started to be developed at the end of the 19th century and the beginning of the 20th century. Since then, a lot of progress has been done, leading to many theoretical consequences and practical applications.

In this thesis we address some problems related to a key property of Quantum Mechanics, entanglement, and to some of the mathematical objects which are believed to capture how this entanglement shows up in many cases in condensed-matter systems, Projected Entangled Pair States. The problems we tackle come from a variety of questions, all related to fundamental questions and tasks in quantum foundations, quantum protocols and quantum many-body physics. Which states can be transformed into others by two parties in two distant places which can communicate only classicaly? Which is the relationship between the uncertainty inherent to different quantum measurements and the non-classical correlations which may appear in the corresponding set of outcomes? And, finally, which is the relationship between states and Hamiltonians in the problem of classifying quantum phases of matter?

In order to deal with these problems we use diverse mathematical techniques, such as symmetric bases, rearrengement invariant spaces, semidefinite programming, spectral theory of bounded and unbounded positive operators, etc. We obtain diverse results both in Mathematics and Physics, and some of these results have already been published in impact ranked peer-reviewed journals.

This memory is structured in five chapters besides this introductory chapter, in which we summarize the problems we tackle, the objects we deal with, the techniques we use and the results we get. The second chapter provides a brief review of some fundamentals of the quantum formalism, leaving specific parts of the needed concepts for each chapter of this work. Each of the subsequent chapters deals with one of the problems we address, comprising the specific definitions and tools needed for solving the problem and the detailed results.

The first problem we solve in this work came up when studying which states could be transformed into others by two distant parties by using local operations and classical communication when some additional resources such as catalysts are allowed. The composite system which results when two different parties are considered is described by the tensor product of the individual systems. The study of such relations involves symmetric and multiplicative structures in tensor products, leading us to the following mathematical questions: Given X and Y with symmetric bases $\{x_i\}_{i=1}^{\infty}$ and $\{y_i\}_{i=1}^{\infty}$, which conditions on the tensor norm α would make $\{x_i \otimes y_j\}_{i,j=1}^{\infty}$ a symmetric basis of $X \hat{\otimes}_\alpha Y$? And, more generally, given two rearrangement invariant spaces X and Y, and given $X \otimes_\alpha Y$ for a tensor norm α, which conditions on α would make its completion $X\hat{\otimes}_\alpha Y$ also a rearrangement invariant space? We treat this problem in the third chapter of this memory, entitled *Rearrangement invariant structures in tensor products*, reaching a characterization for ℓ_p – and c_0 – and L_p spaces in these terms.

In the second problem we characterize which measurements can be jointly measured. Since Heisenberg's Uncertainty Principle, it is known that there are some magnitudes that cannot be determined jointly with accuracy: The sharper one of them is measured, the more undetermined the calculations for the other will result. Projective measurements are known to be jointly measurable if and only if their associated observables commute. However, for generalized measurements no condition was known beyond the case of qubits. We give a computable characterizacion in terms of the quantum correlations that could be exposed by these measurements by calculating the maximal possible violation of Bell inequalities attainable if one of the involved parties uses these measurements. This relates two central concepts in Quantum Theory: Uncertainty Principle and non-locality of Nature. The mathematical tools we use range from semidefinite programming, in both its primal and dual forms, to convexity arguments. The fourth chapter of this memory, *Joint measurability and Bell inequalities*, details the contents of this problem.

The last problem we deal with is related to states and Hamiltonians. Hamiltonians are the energy observables governing the dynamics of systems, and they are determined by the interactions present in the systems. Quantum effects mostly appear when the system is at a very low temperature. At zero temperature the system stabilizes in its *ground state*, which is the eigenvector corresponding to the minimal eigenvalue of the Hamiltonian. It is on this state on which one can perform measurements and observe the *physical properties* of the system. When the temperature is extremely low but not zero, low-lying excitations – i.e. states with low energy – also play a role. This close connection between Hamiltonians – interactions – and ground states makes us analyze the question: Given a quantum state, how many different Hamiltonians, and with which properties, have this state as a ground state. We focus on the case of Projected Entangled Pair States (PEPSs), which are believed to capture the physics of systems with local interactions. For these states, there is a natural way of associating a Hamiltonian: the parent Hamiltonian. We study how robust this construction is: Do small perturbations of the tensor description lead to small perturbations of the associated parent Hamiltonians? We focus on the one-dimensional and two-dimensional cases: Matrix Product States (MPSs) and two-dimensional PEPSs, in the first case in full generality and in the second one via a paradigmatic example, Kitaev's toric code. In the case of MPSs – in Chapter 5 – we show in which cases this construction is robust under perturbation of the matrices which describe the states. Whenever this is not the case, we construct a new family of Hamiltonians – the *uncle Hamiltonians* – as the limit of the perturbed parent Hamiltonians and study their properties: they have the same ground space as the parent Hamiltonian and they are also frustration free. However, they are *gapless* whereas the parent Hamiltonian is *gapped*. In the case of Kitaev's toric code we construct the uncle Hamiltonian for a particular perturbation; the sixth chapter is dedicated to this construction. The mathematical tools we use are mainly spectral results of bounded and unbounded self-adjoint operators, relating results on finite and infinite chains of particles.

1.1. Rearrangement invariant structures in tensor products.

Motivation. When studying some problems in quantum information the first step is to clarify the paradigm we will be working with. Will we have limited amount of memory or infinite? Will we allow quantum communication, just classical communicacion, just some communication conditioned to determined stages of the task? Will different parties share some given quantum resources or some shared randomness? Many other questions can be posed, which can completely change the problem we are dealing with.

Among these paradigms, the setting called 'local operations and classical communication' (LOCC) has been one of the most extensively studied and used scenarios, as the paradigm modelling what can be effectively achieved by two distant laboratories. Given two systems A and B representing those two distant parties, usually called Alice and Bob, only local quantum operations at A and B are allowed and no global operation at $A \otimes B$ can be performed. This means that every operation we perform must be a product operation $U \otimes V$ in case of unitary evolutions, and any measurement must be of the form $\{P_i \otimes Q_j\}_{i,j}$ for $\{P_i\}_i$ and $\{Q_j\}_j$ measurements in Alice's and Bob's sites respectively. The other feature is that unlimited classical communication is allowed – as many rounds as needed – but no quantum resource can be trasmitted between Alice and Bob.

In this setting, one important question in which the role of entanglement is crucial is the following: Given a state shared by Alice and Bob, which states could they get from it? This scenario and this question have motivated two very important measures of entanglement: entanglement of formation and distillable entanglement [**17**]. The first one is related to how many EPRs (bipartite maximally entangled states, e.g. $(|00\rangle + |11\rangle)/\sqrt{2}$) are needed to create a given state by LOCC, while the second one tells us how many EPRs we can get from a given state by LOCC, in both cases in the asymptotic regime.

These measures of entanglement and LOCC convertibility arise from seeing entanglement as a resource for communication. EPR pairs allow some operations that cannot be performed only with classical communication, such as quantum teleportation [**16**], quantum key distribution [**38**], superdense coding [**18**] and improved strategies in interactive proof systems [**65, 69**]. Therefore, if a state can be converted using LOCC into another, the former is more resourceful and more entangled than the latter. Two states that can be mutually converted into each other by just using local unitaries (LU equivalence) have exactly the same type of entanglement, but the additional unlimited use of classical communication in the LOCC setting is considered due to its operational applications.

The problem in bipartite pure states is rather well known. First it was proved that, even though many rounds of classical communication is allowed in this setting, just one round of one-way communication is enough, as shown by Lo and Popescu in [**78**]. Nielsen proved in [**90**] that the key of LOCC convertibilitly lies on the Schmidt coefficients of the states. Given two pure states $|\varphi_1\rangle, |\varphi_2\rangle \in A \otimes B$, with eigenvalues of the respective reduced density matrices $\bar{\lambda} = (\lambda_1, \ldots, \lambda_n)$, $\bar{\mu} = (\mu_1, \ldots, \mu_n)$, it would be possible to transform $|\varphi_1\rangle$ into $|\varphi_2\rangle$ by LOCC iff $\bar{\lambda}$ is majorized by $\bar{\mu}$ (or $\bar{\mu}$ majorizes $\bar{\lambda}$):

$$\sum_{i=1}^{k} \lambda_i^* \leq \sum_{i=1}^{k} \mu_i^*, \ \forall k$$

where $\bar{\lambda}^*$ and $\bar{\mu}^*$ are the respective decreasing rearrangements of $\bar{\lambda}$ and $\bar{\mu}$. In this case we write $|\varphi_1\rangle \to |\varphi_2\rangle$.

Some variations of this problem have been also studied. Jonathan and Plenio [**64**] found that even though $|\varphi_1\rangle$ cannot be converted into $|\varphi_2\rangle$, surprisingly there may exist another state $|c\rangle \in A \otimes B$, called catalyst, that can make this conversion possible: $|\varphi_1\rangle \otimes |c\rangle$ into $|\varphi_2\rangle \otimes |c\rangle$. The catalyst needs to be entangled, which is the reason why this setting is called entanglement-assisted LOCC or ELOCC.

Bandyopadhyay, Roychowdhury and Sun [**14**] showed another surprising fact: it may be possible that $|\varphi_1\rangle$ cannot be converted into $|\varphi_2\rangle$, but $|\varphi_1\rangle^{\otimes n}$ can be converted into $|\varphi_2\rangle^{\otimes n}$ for some number of copies n. This problem is called MLOCC , standing for multiple-copy LOCC.

In [**10**] Aubrun and Nechita characterized both MLOCC and ELOCC majorization: $|\varphi_1\rangle$ can be almost converted into $|\varphi_2\rangle$ by either MLOCC or ELOCC iff $\|\bar{\lambda}\|_p \leq \|\bar{\mu}\|_p$ $\forall p \geq 1$. This 'almost' comes from those states for which the catalysts need to be infinite dimensional, and therefore they characterize the closure of the set of vectors which can be converted into a given one.

Note that MLOCC and ELOCC settings require any characterization to be based on symmetric tools, since the order of the eigenvalues plays no role, and also on multiplicative tools. Therefore, the study of catalysis, its relation with tensor products and symmetric norms, and the MLOCC and ELOCC scenarios led us to the following question: Are the conditions given by Aubrun and Nechita determined by the symmetric and multiplitativite features of MLOCC and ELOCC, or must other additional properties be considered in order to reach this conclussion? Consequently, the problem we tackle initially in this chapter is:

> Given two spaces X and Y with symmetric bases, when is the product basis in $X\hat{\otimes}_\alpha Y$ a symmetric basis for some crossnorm α?

In the case symmetry and multiplicativity characterize ELOCC and MLOCC convertibility, we should get the family of spaces ℓ_p as the only possible result for this last question, and this is indeed the case. We prove that X and Y must be essentially the same space, and they must be an ℓ_p, $1 \leq p < \infty$, or c_0. Aubrun and Nechita also proved later [**11**], with the same type of techniques they used to prove the characterization of MLOCC and ELOCC majorization, the same result concerning bases.

We also extend the result to rearrangment invariant (r.i.) spaces. Therefore, symmetric bases on Banach spaces and r.i. spaces will be the main tools we use for this problem.

Despite this deep knowledge of the pure bipartite scenario, in the mixed bipartite and multipartite settings the LOCC problem is not yet understood. A characterization of LOCC convertibility has not been found, even though there are some partial results towards this aim. Kraus characterized the locally unitarily (LU) equivalence of pure multipartite states [**70**], which is contained in the LOCC class and determines the minimal set of operations under which any multipartite entanglement measure must be invariant.

And de Vicente et al. characterized in **[131]** the 3-qubit entanglement via operational entanglement measurements, and related the classfication they got to the LOCC scenario.

Another setting which has been studied, due to the probabilistic nature inherent to Quantum Mechanics, is stochastic LOCC or SLOCC conversion, in which one must study whether a state can be converted into another with some probability of success **[37]**. Vidal showed that, in the single copy scenario for bipartite pure states, this conversion is possible if and only if the Schmidt rank of the state we have is higher or equal than the Schmidt rank of the state we want to get **[132]**, providing a simple formula that gives the optimal probability of conversion. There are also remarkable results for SLOCC convertibility of mixed states **[66, 75, 127, 128]** and in the pure tripartite setting, as **[28]**, in which the NP-hardness of this problem is found based on its connection to algebraic complexity problems by means of the Schmidt rank. This connection has attracted much attention, as it could be a very promising tool linking these two fields.

Symmetric bases. An early result studying the behaviour of product basis in tensor products of spaces with basis is **[48]**, in which Gelbaum y Lamadrid showed that for any given X and Y, with bases $\{x_n\}$ and $\{y_m\}$, the product basis $\{x_n \otimes y_m\}$ with certain order among the element is a basis of the completed space $X\hat{\otimes}_\alpha Y$ for every uniform crossnorm α.

Another cornerstone in this context is Pisier-Schütt theorem, proven separately by them **[106, 118]**. A slightly weaker version of it could be that if the tensor product of two spaces, both with unconditional bases, completed with respect to a tensor norm has an unconditional basis, then necessarily the product basis is also an unconditional basis.

Unconditionalty in tensor products is a very active research line. In opposition, there exist very few results about symmetric bases in tensor products. The only known works relating symmetric bases and tensor products, as far as we know, are **[117]** by Schütt and **[108]** by Read. In the first one the author proved that the symmetric constant of $\ell_p^n \otimes_{\Delta_r} \ell_r^n$ is not bounded in the dimension n for $1 \leq p, r < 2,\ p \neq r$, and in the second one a particular space E is constructed such that E and $E\hat{\otimes}_\beta E$ are isomorphic for a concrete crossnorm β, but they are not isomorphic as lattices with respect to the usual bases.

Rearrangement invariant spaces. We posed a similar question trying to extend the result to rearrangement invariant (r.i.) spaces: Given two r.i. spaces $X(\Omega_1)$ and $Y(\Omega_2)$, in which cases do we have $X(\Omega_1)\hat{\otimes}_\alpha Y(\Omega_2) = Z(\Omega_1 \times \Omega_2)$ for some r.i. space Z and some crossnorm α?

The connections between tensor products and rearrangement invariant Banach spaces have been studied in several works – see for instance **[82, 93]** and the references therein. The general framework has been the following: Let $X(\Omega_1)$, $Y(\Omega_2)$ and $Z(\Omega_1 \times \Omega_2)$ be Banach function spaces. In which cases is the bilinear operator

$$B : X(\Omega_1) \times Y(\Omega_2) \longrightarrow Z(\Omega_1 \times \Omega_2),$$

defined as $B(x,y)(s,t) = x \otimes y(s,t) = x(s)y(t)$ for every $(s,t) \in \Omega_1 \times \Omega_2$, bounded? Or, equivalently, when do we have a continuous embedding $X(\Omega_1)\hat{\otimes}_\pi Y(\Omega_2) \subseteq Z(\Omega_1 \times \Omega_2)$? Here, π denotes the projective tensor norm on $X(\Omega_1) \otimes Y(\Omega_2)$ and $X(\Omega_1)\hat{\otimes}_\pi Y(\Omega_2)$ the completion of $(X(\Omega_1)\otimes Y(\Omega_2), \|\cdot\|_\pi)$.

The close connection between the continuity of the operator B and the stability problem of the integral operator – see [**82**], Part III – has motivated a deep research on this problem. Most of these works (see for instance [**5, 83, 84, 85, 93, 121**]) have focused their results on concrete and important spaces: Lorentz spaces, Orlicz spaces, Marcinkiewicz spaces and so on.

More recently, in [**8**], this problem was studied on the general context of symmetric function spaces on [0,1]. The tensor product was there used to study the multiplicator space $\mathcal{M}(X)$ of X. In [**9**] the authors focused their work on rearrangement invariant (r.i.) Banach spaces on $[0,1]$, relating the multiplicator space $\mathcal{M}(X)$ with properties of subspaces of X and, again, with the continuity of the multiplication operator B.

A priori, there can be 'many' r.i. structures on the same space $X(\Omega_1)\hat{\otimes}_\alpha Y(\Omega_2)$. Nevertheless, there exists a 'natural' structure on $\Omega_1\times\Omega_2$ associated to the product operator B. We are asking thus about the cases in which $X(\Omega_1)\hat{\otimes}_\alpha Y(\Omega_2) = Z(\Omega_1\times\Omega_2)$, for some r.i. space Z.

Thus, we will be interested in the cases in which the operator B is not only continuous, but also a topological isomorphism.

Finally, it is worth mentioning that there is another line of study relating tensor products and ordered structures. In [**45**] and [**46**], the author started a research about the possibility of defining crossnorms on tensor products of Banach lattices in such a way that they preserve the lattice structure (see also [**35**]). A lot of work has been done in this direction, but the symmetric structure inherent to r.i. spaces makes our problem much more restrictive.

Main results. For the problem in symmetric bases[1], the result stems on a characterizacion of the spaces ℓ_p and c_0 given by Altshuler in [**3**]: Given a space X with symmetric basis $\{e_i\}$, X is isomorphic to c_0 or some ℓ_p if and only if for every $a=\sum_{i=1}^\infty a_ie_i$, $b=\sum_{j=1}^\infty b_je_j$, $a,b\in X$, and every set of disjoint sequences of the basis $\{(e_{i,j})_{j=1}^\infty,\ i\in\mathbb{N}\}$, there must exists a constant $K>0$ such that

$$K^{-1}\|a\|\cdot\|b\| \le \Big\|\sum_{i,j=1}^\infty a_ib_je_{i,j}\Big\| \le K\|a\|\cdot\|b\| \ .$$

This let us proof our first result:

THEOREM. *If X, Y are spaces with symmetric bases $\{x_n\}_{n=1}^\infty$ and $\{y_n\}_{n=1}^\infty$ respectively, such that there exists a crossnorm α that makes $\{x_n\otimes y_m\}_{n,m=1}^\infty$ a symmetric basis in $Z=X\hat{\otimes}_\alpha Y$, then $X=Y=Z$ is the space ℓ_p and $\alpha=\Delta_p$ for some $1\le p<\infty$, or it is the space c_0 and $\alpha=\varepsilon$.*

[1]Note this excludes ℓ_∞, therefore when we refer to some ℓ_p, it is for $1\le p<\infty$.

Regarding the problem in rearrangement invariant spaces we use two previous results from Ashtaskin et al. in [**9**] and Hernández et al. in [**62**] in order to prove our second result:

THEOREM. *Let X, Y, Z be r.i. spaces on $\Omega = [0,1]$ or $[0,\infty)$, such that the multiplication operator*

$$B : X(\Omega) \otimes_\alpha Y(\Omega) \longrightarrow Z(\Omega \times \Omega),$$

defined as $B(x \otimes y)(s,t) = x(s)y(t)$ for every $(s,t) \in \Omega \times \Omega$, is bounded. Then B can be extended to a topological isomorphism $\hat{B}$ from $X(\Omega)\hat{\otimes}_\alpha Y(\Omega)$ onto $Z(\Omega \times \Omega)$ if and only if there exists a $p \in [1,\infty)$ such that $X = Y = Z = L_p$ and $\alpha = \Delta_p$.

We also briefly discuss the optimality of the first result, in the sense that no Pisier-Schütt type theorem can be stated in this context, showing the previously mentioned example by Read [**108**], and another by Pełczyński [**99**], of spaces X with symmetric basis and a crossnorm β such that $X\hat{\otimes}_\beta X$ have also a symmetric basis but their product bases are not symmetric.

1.2. Joint measurability and Bell inequalities.

Motivation. One of the most striking consequences of Quantum Mechanichs is the non-locality of Nature, first posed by Einstein, Podolski and Rosen in [**39**] in 1935. If two distant parties perform certain measurements on entangled states, the outcomes they get may show certain correlations that cannot be explained by the classical laws of physics. This 'magic' behaviour of matter was at first thought as a lack of completeness of quantum theory.

However, every physical theory that could be a refinement of Quantum Mechanincs would still show this strange behaviour. Thirty years later, Bell proposed an experiment [**15**] which would validate the existence of these correlations and thus give evidences for the quantum theory to be definitely accepted. In his experiment every output coming from 'classical behaviours' of Nature would be bounded by some value, but some quantum states (in the case they existed) would make this inequality be violated.

This experimental proof is taken for granted nowadays, and the disbelief in Quantum Mechanics has been almost completely removed. The interest on non-locality is also very high in the quantum information community, due to the many applications this phenomenon leads to, ranging from quantum cryptography [**38, 104, 124**] to randomness amplification [**31**], as well as its theoretical implications in foundations of Physics.

It is known that not every quantum experiment can lead to strictly quantum probability distributions. On the one hand, it depends on the bipartite state, as non entangled states and even some entangled ones always give probabilites with a 'classical explanation'. On the other hand, it also depends on the measurements used in the experiment, since it is known, for example, that jointly measurable observables can never lead to violations of Bell inequalities.

The opposite question, whether non-jointly measurable observables can always lead to some Bell type violation, has hardly been addressed, and it is the one we characterize in this chapter. For projective measurements it is well known that joint measurability and commutativity are equivalent, but for generalized measurements (POVMs) no criterion was known beyond two-level systems. The main tool in this analysis will be the identification of the CHSH inequality with the Lagrangian dual of the joint measurability problem. This connection allows us at the same time to provide simple criteria for joint measurability.

The main consequence of the results in this chapter is a relationship never found before between two major ingredients of quantum theory: the existence of magnitudes that cannot be measured jointly and the violation of Bell inequalities. We can conclude that measurements that cannot be measured jointly in Quantum Mechanics cannot be measured jointly in any other no-signalling theory.

Non-locality and Bell inequalities, and no-signalling. In the paper Einstein, Podolski and Rosen published together in 1935, they proposed a theoretical experiment that could lead to a possible incompleteness of Quantum Mechanics. Given that two particles could 'share' conjugate magnitudes, one could be able to measure 'simultaneously' one of this magnitudes in the first of the particles, and the other in the second. This way, one would break Heisenberg's Uncertainty Principle. They concluded that there should exist more 'elements or reality' that would determine these magnitudes, even though we could not have control over them. Such models are usually called local hidden variables (LHV).

The other possible explanation would be admitting the non-locality of Nature, allowing 'spooky actions at a distance' being possible. When measuring one of the particles, the other would be automatically transformed by the action onto the first, and therefore the second magnitude would not be measured correctly. Heisenberg's Principle would not be broken in this case, but the payout is large; not everyone felt comfortable with this possible instantaneous actions at distant places.

In 1964, Bell proposed a simple experiment that would certificate this possible non-local behaviour of Nature. However, physical devices have not yet been able to fully test this option. Indeed, there still exist some problems to definitely assess the existence of these non-local behaviours, mainly due to the non-perfect eficiency of detectors, the so-called detection loophole [**7, 98**].

One can distinguish among several types of probability distributions coming from experiments. In the first place, we have those that could be explained by LHV models; they form a polytope, and distributions coming from such models are called classical distributions or classical behaviours, because they can be expressed as convex combinations of classical distributions in the usual sense. The second set, including the latter, is the set of probability distributions coming from quantum experiments; they no longer form a polytope but it is still convex. There exists a third interesting larger set – also a polytope

– , consisting of the so-called no-signalling distributions, comprising all distributions for which the only assumption is that no information can travel faster than the speed of light. Other sets have been studied – see for instance [**88**] –, depending on the physical assumptions different theories could have.

The hyperplanes which delimit the set of classical behaviours give rise to inequalities corresponding to the respective semispaces in which classical distributions lie. These inequalities are called Bell inequalities, and the difference between classical and quantum behaviours can be witnessed by a Bell inequality violation. The very best known example is CHSH [**30**], which requires two measurements with two outcomes each.

The study of Bell inequalities is a very active research line, and have led to very interesting results, ranging from Tsirelson bounds [**122**], to the possibility of unbounded violation of Bell inequalities in the tripartite setting [**102**], and many others. They have also been proposed as an entanglement measure, and for countless applications. In this line, CHSH rigidity have led to its application for device-independent quantum cryptography [**110**]. Additionally, non-locality has been identified as a requirement for quantum key distribution [**12**], for secure randomness generation [**105**] or as a resource for better strategies in quantum games [**40, 81**].

Even though entanglement is a necessary resource for an experiment to exhibit quantum non-localitly, it has been shown that some entangled states, called bound-entangled states, would never show any non-local behaviour. On the contrary, another requirement for an experiment to show a non-local behaviour is that measurements are not jointly measurable, and in this work we show that the converse is also true: whenever two measurements cannot be measured jointly, they can be used to design an experiment which leads to a Bell violation for some quantum state.

As a result, we also link joint measurability in Quantum Mechanics with joint measurability in any no-signalling theory compatible with Quantum Theory.

Joint measurability. Heisenberg's Uncertainty Principle is another fundamental consequence of Quantum Mechanics. It states that there exist conjugate magnitudes that cannot be measured jointly with accuracy. The more precise we determine one of them, the more imprecise the information we obtain about the other will be. This is, in part, a consequence of the fact that measuring a particle modifies it, which prevents from measuring the first magnitude and afterwards the second one.

It is known that for a family of commuting 'sharp' observables – coming from simultaneously diagonalizable Hermitian operators whose eigenspaces determine the projective measurements –, another 'sharp' observable can be found so that the information of the original family can be recovered. And in the opposite direction, two such observables cannot be jointly measured if they do not commute.

For generalized measurements – also called positive operator valued measurements or POVMs –, in which we do not have control of the whole system for performing projections, this equivalence is no longer true. Starting from commuting POVMs we can always build another POVM that implements them all together, but there also exist non-commuting generalized measurements that can likewise be performed jointly by another POVM.

The aim of this chapter is to give characterizations of the non-joint measurability of these generalized measurements from different perspectives: as a majorization problem among – semidefinite – positive operators, as an optimization problem, and finally by using them to violate a Bell inequality. There exists not much previous work about this issue. No previous criterion for joint measurability of POVMs was known beyond two-level systems [**24, 119, 137**], and in [**4**] it was observed that the border of joint measurability coincides with the one for CHSH violation for particular two-level observables.

There exist more notions related to joint measurability that have been studied, such as coexistence of effects [**109**], non-disturbance [**61, 96**], compatibility and strong compatibility [**59**], and other problems related to ours, such us informationally complete joint measurements [**25**] and simultaneous approximation of incompatible measurements [**58**].

Semidefinite programming. The last tool we use is semidefinite programming, as the first characterization we get for jointly measurable observables can be translated into a semidefinite programming problem.

Semidefinite programming (SDP) is a class of convex optimization problems, including, among many others, linear programming. They have a linear function as objective function and a feasible affine set determined by inequalities among semidefinite positive matrices.

SDP belongs to the class of polynomial approximable problems under some conditions for which the problems are well-behaved [**47**], and it has proven very useful in the design of approximating algorithms for some classical NP-hard problems, yielding better approximations than previous lineal programming approximations. In this line, SDP has led to many results in combinatorial complexity, such as exact polynomial time algorithms for colouring perfect graphs, tractable bounds for the Shannon capacity of graphs, and the best known approximations for max-cut, graph partitioning, and discrepancy minimization. In Quantum Information, SDP has also been applied to many problems, leading to very interesting results, such as approximations of the classical value of non-local XOR games – together with Tsirelson bounds for these values – and approximations of quantum values of non-local games and quantum problems in graphs – via a hierarchy of SPD relaxations.

We also make use of the fact that the Langrangian dual of any SPD problem is also in the SPD class, which attains the same optimum in the case the first problem attains its optimum – due to strong duality. This lets us relate the joint measurability problem with the violation of a CHSH-type Bell inequality.

Main results. We first focus on the problem of joint measurability of two dichotomic – two outcomes – observables. Each of them can be decomposed into two positive operators P and $\mathbb{I}-P$, called effects. Then we translate the needed conditions to a majorization problem among semidefinite positive operators.

Proposition. *Two observables characterized by effect P and Q are jointly measurable iff there exists a positive semidefinite operator S satisfying $Q + P - \mathbb{I} \leq S \leq P, Q$.*

A semidefinite positive operator S such that $S \leq P, Q$ always exists – $S = 0$ –, which let us state an equivalent optimization problem, with non-empty feasible set, by calculating the minimum λ such that $Q + P - \lambda\mathbb{I} \leq S \leq P, Q$ for any semidefinite positive S.

Proposition. *Two observables described by effect operators P and Q are jointly measureable iff the solution of the semidefinite program*

$$\lambda_0 = \inf\{\lambda \in \mathbb{R},\ \ Q + P \leq \lambda\mathbb{I} + S\},$$

subject to $0 \leq S \leq Q, P$, is lower or equal to 1.

Taking the dual and modifying it allows us to rephrase the problem in terms of the violation of a CHSH-type inequality for some quantum state.

Theorem. *Two observables determined by effect operators P and Q are not jointly measureable iff they enable the violation of a CHSH inequality. Quantitetively, there exist B_1 and B_2 dichotomic ± 1 valued POVMs such that the supremum of expectation value of the CHSH operator*

$$\mathbb{B} = (A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2))/2,$$

for $A_1 = \mathbb{I} - 2P$ and $A_2 = 2Q - \mathbb{I}$, over all possible quantum states is

$$\sup_\rho \left|\langle \mathbb{B}_\rho \rangle\right| = 1 + 2\lambda_0^*,$$

whereas $\left|\langle \mathbb{B}_\rho \rangle\right| \leq 1$ for every separable state ρ.

Additionally, we give a computable characterization of joint measurability of POVMs.

Theorem. *The supremum can be computed by calculating $\lambda_0^* = \max_{\phi \in [0,\pi]} \mu(\phi)$ where $\mu(\phi)$ is the largest eigenvalue of*

$$(Q + P - \mathbb{I}) \otimes \begin{pmatrix} c^2 & cs \\ cs & s^2 \end{pmatrix} - Q \oplus P,$$

with $c = \cos(\phi)$ and $s = \sin(\phi)$.

Finally, we link the previous results to the no-signalling scenario, since the CHSH violation characterization implies that the observables would still be non-jointly measurable in any no-signalling theory.

We also briefly discuss the cases of more dichotomic observables, and observables with more than two outcomes.

1.3. Uncle Hamiltonians for Matrix Product States.

Motivation. In multipartite systems, entanglement gets more complicated than in bipartite systems, depending on the partitions we set. Whenever we consider the space separated in more than two regions, there is no standard way of quantifying entanglement, nor equivalent operations to distillation or dilution. In the tripartite case, the W-state and the GHZ-state,

$$|\mathrm{W}\rangle = \frac{|001\rangle + |010\rangle + |100\rangle}{\sqrt{3}}, \; |\mathrm{GHZ}\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}},$$

are a perfect example of this fact **[37]**. However, when we consider just two regions, there are many applications of the study of the entropy of entaglement to the context of many-body physics.

Most of the systems in equilibrium that appear in Nature exhibit a particular interesting property at zero temperature: An area law for the entropy of entanglement between two disjoint regions. That is, the entropy of entanglement depends on the size of the boundary separating the two regions instead of depending on the whole bulk, which is the case for generic random states.

In one-dimensional lattices, Matrix Product States (MPSs), initially known as finitely correlated states **[41]**, are a family of states which is perfectly suited to tackle problems in these settings. They seem to capture the physics of local interactions in one-dimensional systems.

From the numerical point of view, MPSs are the variational set for very successful methods based on renormalization group methods. Matrix Product States just need a few parameters, and help overcome the problem of dealing with the exponential many parameters generic states need to be described. Their ability to approximate 'natural' states has been supported by many theoretical results, such as Hasting's results relating ground states of gapped Hamiltonians to the area law and states with exponential decay of correlations, and Brandao and Horodecki's result relating this exponential decay of correlations to MPSs.

MPSs have also proven useful in the problem of classifying all phases of matter in one dimension and in clarifying the role of symmetries and their connection to string order parameters. In order to achieve such results, it has been crucial to have a Hamiltonian which can be naturally associated to every MPS: the parent Hamiltonian, which has the MPS as ground state. Hamiltonians, which encode interactions in systems, govern the evolution of such systems. At zero temperature these systems stay in the so-called ground states, which are the eigenstates associated to the minimal eigenvalues of the Hamiltonians, and on which one can *measure* the physical properties of the system.

Given a Hamiltonian, its ground states are determined. On the other hand, for a given state, there can be many different Hamiltonians which have this state as ground state. This fact is what motivated the following questions: How robust is the parent Hamiltonian construction for a given MPS? And, may there exist other Hamiltonians for a given

MPS which show different properties than the ones from the parent Hamiltonian?

This is the scope of this chapter. We consider the parent Hamiltonians corresponding to small perturbations of a given Matrix Product State and consider the limit when the perturbation vanishes. Whenever this limit is different from the parent Hamitolnian of the original MPS – when the MPS is non-injective–, the new Hamiltonian is termed 'uncle Hamiltonian', whose properties – ground state space and spectrum – we study. We find that both parent and uncle Hamiltonians share the ground space in the case of non-injective Matrix Product States, and the uncle Hamiltonian is gapless whereas the parent Hamiltonian is gapped. We study both cases of finite chains and infinite chains – the thermodynamic limit. For injective MPSs, we use a non-injective description to construct gapless uncle Hamiltonians, but in this case the ground space for finite chains does not coincide with the one from the parent Hamiltonian.

Matrix Product States. The description of a generic state from a system consisting of a large number n of particles is very complicated. If each particle can be described by a d-dimensional Hilbert space, the composite system is described by a d^n-dimensional Hilbert space. Therefore, we would need to gain control of an exponential number of parameters in order to be able to perform any type of calculation as systems grow.

Fortunately, natural interactions are highly local, and therefore those states effectively arising are only a small fraction from the whole set of states at which a composite system could be. For systems in one-dimensional lattices, this property of Nature seems to be well captured by the so-called Matrix Product States, which are states whose coefficients can be described by some sets of matrices $\{A_i^{[k]},\ i=1,\dots,d,\ k=1,\dots,n\}$ as

$$|\varphi\rangle = \sum_{i_j=1}^{d} \operatorname{tr}(XA_{i_1}^{[1]}A_{i_2}^{[2]}\cdots A_{i_3}^{[3]})|i_1 i_2 \dots i_n\rangle \ ,$$

where the matrix X encodes the boundary conditions, either pure – $X=|r\rangle\langle l|$ – or mixed.

Indeed, every state can be described as a Matrix Product State if the matrix dimensions are taken large enough, by taking sucessive Schmidt decompositions of the state and storing the coefficients in suitable matrices. However, dealing with such descriptions could be even worse than trying to manage the coefficients of the states directly. On the other hand, MPSs let us efficiently approximate those 'natural' states aforementioned.

Locality of Nature, implying that systems are governed by local interactions and local Hamiltonians, makes physically relevant states satisfy some special properties: they usually show fast decaying two-points correlations and they exhibit what is called an area law for the entanglement entropy, that is, given a separating cut in the system, the entropy of entanglement depends on the length of this cut instead of on the size of the two regions delimited by this cut. Matrix Product States satisfy this area law, since the entropy of entanglement is controlled by the dimension of the matrices adjacent to the cut.

The relationship among ground states of local Hamiltonians, this area law and the rate at which correlations decay in those states has been the object of study in many works.

Hastings proved in [**57**] that ground states of gapped[2] local Hamiltonians have exponential decay of correlations, and in [**19**] it was shown that states in one-dimensional chains showing exponential decay of correlations can be well approximated by MPSs, improving a previous result of Hastings [**56**], where he demanded the state to be a ground state of gapped local Hamiltonian. Some of the latest results completing this picture include [**6**], which improved exponentially the parameters in [**56**], and [**72**], in which the authors gave a randomized polynomial-time algorithm for approximating ground states of gapped one-dimensional Hamiltonians.

All these results go far beyond their theoretical implications, since they support the good performance of numerical methods based on renormalization group techniques, for which MPSs are an essential tool [**92, 111, 129**].

In addition, not only are MPSs a good tool to efficiently describe one-dimensional ground states approximately, they also describe exactly many interesting states such as GHZ states [**49**], W-states [**37**], 1D-cluster states [**22**], AKLT states [**1**], and others, with low dimensional matrices. MPSs have also proven useful to describe sequentially generated states [**113**], and to perform tasks in measurement-based quantum computation [**50**].

MPSs – capturing the physics of 1D systems – have also led to interesting theoretical results, such us the role of symmetries in spin chains [**114**] and the classification of gapped quantum phases on 1D systems in [**27, 42, 107, 115**].

MPSs can be extended to higher dimensional lattices to the so-called Projected Entangled Pair States (PEPSs, [**126**]). Even though PEPSs do not have the strong theoretical support MPSs do in relation to the problem of approximating ground states – we could highlight [**55**] among those supporting it –, they have also proven to be a very good tool for numerical purposes [**95**] and they have led to many theoretical and applied results, due to the link between their properties and the lattice in which they are defined. We also deal, in another chapter, with the case of 2-dimensional lattices, focusing on one of the paradigmatic examples: the toric code [**67**].

Associated Hamiltonians. As we just mentioned, MPSs efficiently approximate ground states of gapped[3] local Hamiltonians and describe exactly, with low bond dimension, many interesting states.

In the other direction, every MPS can be found to be an exact ground state of a local Hamiltonian. One of these local Hamiltonians is called parent Hamiltonian [**41, 101**], whose local terms are orthogonal proyectors. Under a quite general condition, called injectivity, the parent Hamiltonian is gapped and has the corresponding MPS as its unique ground state. Moreover, for translationally invariant MPSs, the normal form found by Pérez-García et al. in [**101**] clearly determines the dimension of the ground state space, depending on its injectivity or block-injectivity. Parent Hamiltonians are one of the main

[2]Later on, different notions of gap will be presented. The notion of gapped Hamiltonian in the results mentioned here is the strongest one of those we mention, with a unique ground state.

[3]Again, strong gap definition.

tools we use in this chapter.

Parent Hamiltonians are determined by the matrix description of the states, therefore defining a mapping[4] from sets of matrices to families of local Hamiltonians,

$$A \mapsto \hat{H}(A) \ .$$

Our purpose is to study the robustness of this construction. That is, will continuous linear perturbations $A + \varepsilon P$ of the matrix description lead to continuous deformations of the parent Hamiltonians? The answer is not always positive, as it was noted in [**26**] for 2-dimensional lattices.

Whenever this last question has a negative answer, we consider the limit Hamiltonians

$$H'_P(A) = \lim_{\varepsilon \to 0} \hat{H}(A + \varepsilon P),$$

which we call 'uncle' Hamiltonians, and for which the MPS described by the set of matrices A is also an exact ground state. We also study their complete ground state space structure, comparing it with the ground state space of the parent Hamiltonians.

We must note that the perturbations induced by this procedure generally not small, therefore the results we present do not contradict at all those from Michalakis and Zwolak [**80**] about stability of local Hamiltonians under small local perturbations.

Spectral gaps and thermodynamic limits. Another fundamental notion of Hamiltonians on lattices is the spectral gap. A family of Hamiltonians, on a finite but growing system, is said to be gapped whenever there exists a uniform bound Δ between the lowest eigenvalue, corresponding to the ground state space, and the rest of energy levels as the length of the system grows. For some applications the definition of gap can also be relaxed, requiring the existence of a uniform bound between several lowest energy levels, which tend to the same limit value – ground space splitting–, and the rest of energy levels; or it can be strenghtened, considering gapless those Hamiltonians whose ground space is not one-dimensional – i.e. degenerate. In our work, we will be considering the former notion of gap.

In connection to the study of spectra for growing chains, one can also study the properties of the Hamiltonians directly on infinite chains, which is called thermodynamic limit in the Physics literature. Its formalization requires some additional tools, such as moving to the Heisenberg picture for observables and dealing with unbounded operators. In this dual picture, the unitary evolution determined by the Hamiltonian of the system acts on the observables instead of on the states, and states act on these observables giving as a result the expectation value of the measurement. This is the point of view of states in the context of C^*-algebras. In this setting, a thermodynamic limit Hamiltonian is said to be gapped if the lowest spectral value is isolated in the spectrum. Again, two different notions of gap can be considered, depending on whether we require the ground state space to be one-dimensional or not.

The notion of gap is crucial in order to classify matter into different phases. Two states are usually defined to be in the same phase whenever there exists a smooth path

[4]Once fixed the considered interaction length.

of gapped Hamiltonians H_λ such that they are respectively ground states of H_0 and H_1 and the gap does not close along the path: $\Delta_\lambda > 0$. Observe that this definition depends on the considered type of spectral gap. The existence of a spectral gap is also important for the protection of the ground state space against physical imperfections [**80**] and for applying efficient algoritms to find the ground state [**72**].

One must be careful when studying Hamiltonian gaps in finite and infinite chains. In finite chains with open boundary conditions, there may exist some boundary effects in the Hamiltonian that stop appearing in the thermodynamic limit [**13, 41**].

Focusing on our problem, all parent Hamiltonians show a spectral gap above the ground state space level – degenerate or not –, and we study this property on the uncle Hamiltonians. Both parent and uncle Hamiltonians have the same ground space, but the uncle Hamiltonian is gapless.

Main results. As we already mentioned, our main purpose is the study of the robustness of the parent Hamiltonian construction and the relationship of states and Hamiltonians for which they are gound states. In the first place, we show that for a given injective tensor A, the perturbation of the tensor induces continuous perturbations of the parent Hamiltonian. Therefore, we focus our study on block-injective tensors, for which we construct the limit uncle Hamiltonians. We detail the results for 2-block-injective tensors, although they can be extended in full generallity to block-injective tensors straightforwardly.

The first property we study is the ground space structure of the uncle Hamiltonians for closed chains, i.e., with periodic boundary conditions, leading to the first result.

THEOREM. *Given a block-injective tensor A describing an MPS with periodic boundary conditions $X = \mathbb{I}$, for almost every*[5] *linear tensor perturbation P the ground space of the uncle Hamiltonian H'_P coincides with the ground space of the original parent Hamiltonian.*

We also give some easily verifiable conditions for the perturbation P so that the uncle Hamiltonian has this property.

The second object we study is the spectral gap of the uncle Hamiltonian on size growing chains, where we get our second result.

THEOREM. *Given a block-injective tensor A describing an MPS with periodic boundary conditions, for almost every linear tensor perturbation P the uncle Hamiltonian H'_P is gapless.*

[5]In this result and the following ones, 'almost every' means that the statement may fail in an algebraic subvariety.

This constrasts with the gapness of the parent Hamiltonian. When we move to the thermodynamic limit we get a similar result.

> THEOREM. *Given a block-injective tensor A describing an MPS, for almost every linear tensor perturbation P the uncle Hamiltonian H_P' is gapless in the thermodynamic limit, and its spectrum is the entire positive real line.*

Given that the spectral gap is a crucial feature in phase classification, these results point out that some precautions must be taken when trying to define this phase classification at the level of states instead of at the level of the interactions that give rise to the Hamiltonians, since the same state can be ground state of Hamiltonians with very different spectral properties which nevertheless have the same ground state space.

Finally, the study of the thermodynamic limit of the uncle Hamiltonian lets us deepen our study of the spectra for finite chains.

> THEOREM. *Given a block-injective tensor A describing an MPS, for almost every linear tensor perturbation P the spectra of the uncle Hamiltonian H_P' on size growing chains tend to be dense in the positive real line.*

We not only study uncle Hamiltonians for block-injective MPSs, but we also construct some uncle Hamiltonians for injective MPSs by taking a non-injective description for them. In this case, the spectral properties above mentioned keep valid, but the ground state space is no longer the same as the one from the parent Hamiltonian for finite chains. In the thermodynamic limit, both ground state spaces coincide: the MPS as the unique ground state.

1.4. Uncle Hamiltonian for the toric code.

Motivation. The generalization of Matrix Product States to higher-dimensional lattices is called Projected Entangled Pair States (PEPSs) [**126**], whose name comes from one of the procedures to construct them: by projecting[6] maximally entangled states along the edges of the lattice, with a mapping determined by a tensor. In the one-dimensional case these tensors can be seen as a set of matrices, therefore the 'Matrix Product' in the name of MPSs ; in the two dimensional case for square lattices the tensors will be 5-index tensors.

PEPSs share many properties with MPSs: they satisfy an area law for the entanglement entropy, they are ground states of local parent Hamiltonians [**100**], they come along with efficient methods to calculate expectation values, they provide exact descriptions of any state for large enough tensors, they describe exactly many interesting states with low bond dimension, they can be used for measurement based – universal in this case – quantum computation [**130**], etc. On the contrary, there exists no normal form for them,

[6]Even though the mapping used to perform such operation is called projection, it is not generally a real projection.

injectivity does not imply that the parent Hamiltonian is gapped [**100**], and they are not yet known to approximate efficiently every ground state of a local gapped Hamiltonian. Despite these facts, they are anyway a very good numerical tool, as many works have shown [**95**]. And, numerical applications aside, PEPSs have provided insight to a very interesting property some systems on two and higher dimensional lattices may show [**114**]: topological order.

The study of topological ordered phases in Condensed Matter Physics began in the 80s with the discovery of the fractional quantum Hall effect and high-temperature superconductivity. In the quantum information community, the attention to topological phases grew after Kitaev posed one of the paradigmatic examples: the toric code. The properties of these families of states make some of them suitable for some applications, such as more robust universal quantum computing or their use as a reliable quantum memory.

In this chapter, as in the previous one, we focus on the relationship between states and Hamiltonians. We work with Kitaev's toric code, its PEPS description, and its related parent Hamiltonian, in order to derive a new gapless Hamiltonian, the uncle Hamiltonian, for which the ground state space is also the toric code.

Toric code and topological order. In [**67**], Kitaev proposed a local Hamiltonian, the toric code, whose properties have led to a whole new paradigm from the quantum information point of view: topological quantum computation. He also generalized this model to the so-called quantum double models.

Kitaev proposed the ground space of this local Hamiltonian and its low-lying excitations as a model where some fault-taulerant computations could be made. Even though it was later shown to have some weaknesses, the properties it had have been extended to other models with many applications in the fields of quantum memories [**2, 21, 33, 51**] and quantum computation [**89**]. The information is stored in this low energy excitations or anyons, which can be seen as quasiparticles, and the gates can be implemented by simply braiding them. These quasiparticles show statistics beyond the bosonic and fermionic types.

Some of these properties depend on the topology of the lattice of the system – as the degeneracy of the ground state space –, and other properties are also intrinsically topological – as the braiding statistics of the anyons –, giving rise to what is called topological order. Additional features include local indistinguishability of ground states, topological corrections to the entanglement entropy area law [**68**], and Hamiltonians showing a spectral gap which is stable against local perturbations.

By examining these properties, one can see that some of them are only related to the states, and some depend on the Hamiltonian for which they are ground states. The relationship among these properties is not very well understood yet. Thus, the question of whether the same states – or family of states – can be ground states of different Hamiltonians with different spectral properties – mainly concerning the spectral gap – becomes important in this setting.

Most of the known topological systems have a description in terms of PEPSs, as shown in [**114**]. There, the authors studied the role of local symmetries in this topological behaviour. PEPSs with such symmetries, and giving rise to such models, are called G-isometric PEPS; the toric code can be modelled as a $\mathbb{Z}_2$-isometric PEPS, as we shall see.

We take advantage of the lack of robustness of the parent Hamiltonian construction under perturbation of the tensor description, as first noted in [**26**], and we extend the tools from the previous chapter to two-dimensional lattices in order to study new Hamiltonians for topological models. We use the paradigmatic toric code, its PEPS description, and this lack of robustness, to construct the *uncle* Hamiltonian for the toric code. This way we show that topological ordered states can also be ground states of gapless Hamiltonians. The lack of a normal form for PEPSs does not allow us to study this problem in full generality, as we have done with MPSs. However, the results shown can be partially extendable to other states, such as Resonating Valence Bond States.

Main results. By taking a particular perturbation of the PEPS description of the toric code, which we take in the orthogonal direction to the projection determined by the toric code PEPS tensor, we consider an uncle Hamiltonian for the toric code. This uncle Hamiltonian is different from the parent Hamiltonian, as shown by every one of its local terms, and has very interesting properties we study and compare to those from the original Hamiltonian.

In the first place, we show that the ground state space of both Hamiltonians coincide for periodic boundary conditions.

THEOREM. *The parent and the uncle Hamiltonian for the toric code have the same ground state space for periodic boundary conditions.*

Secondly, we move to the study of the spectrum. We show that the toric code can also be associated to gapless Hamiltonians.

THEOREM. *The uncle Hamiltonian for the toric code on a finite growing lattice with periodic boundary conditions is gapless.*

These two properties remain true in the thermodynamic limit, no matter whether we allow just one lattice dimension grow or we make them both tend to infinity.

THEOREM. *The uncle Hamiltonian and the parent Hamiltonian for the toric code have the same ground state space in the thermodynamic limit. Even though the parent Hamiltonian is gapped, the uncle Hamiltonian is gapless and its spectrum is the entire positive real line.*

As a final result, and thanks to the study of the thermodynamic limit of the uncle Hamiltonian, we are able to deduce more properties of the uncle Hamiltonian on finite lattices.

THEOREM. *The spectra of the uncle Hamiltonian for the toric code on finite lattices tend to be dense in the positive real line.*

1.5. About this thesis.

This memory is presented by Carlos Fernández González, at the Mathematical Analysis Department of Universidad Complutense de Madrid, in order to opt for the European Degree of Doctor of Philosophy Degree on Mathematics. This work has been conducted under the tuition of Prof. David Pérez García, in the Doctoral Program 'Matemáticas' at the School of Mathematics of Universidad Complutense de Madrid.

During his doctoral period, Carlos Fernández has enjoyed two research stays, at Niels Bohr Institute in Copenhagen with Prof. Michael Wolf, from September 15th to December 15th, 2008, and at the Institute for Quantum Informacion at RWTH-Aachen with Prof. Norbert Schuch, from February 1st to May 1st, 2013. Part of this work was made during these stays. It has also been partially carried out at Centro de Ciencias de Benasque Pedro Pascual, during the Quantum Information Workshop held in June, 2011.

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The work presented here has been partially published in peer-reviewed journals. Three research papers have been accepted and published, comprising respectively the main contents of chapters 3, 4 and 6:

C. Fernández-González, C. Palazuelos and D. Pérez-García, *The natural rearrangement invariant structure on tensor products*, Journal of Mathematical Analysis and Applications **343** 1, 40-47 (2008).

M. M. Wolf, D. Pérez-García, C. Fernandez, *Measurements incompatible in Quantum Theory cannot be measured jointly in any other local theory*, Physical Review Letters **103**, 230402 (2009), arXiv:quant-ph/0905.2998.

C. Fernández-González, N. Schuch, M. M. Wolf, J. I. Cirac, and D. Pérez-García, *Gapless Hamiltonians for the Toric Code Using the Projected Entangled Pair State Formalism*, Physical Review Letters **109**, 260401 (2012), arXiv:quant-ph/1111.5817.

Main contents from Chapter 5 have already been submitted for publication, currently under revision process.

Most of the results have also been presented in different conferences and workshops:

Contributed talks:

La estructura natural de espacio invariante por reordenamiento sobre el producto tensorial, presented in the conference IV Encuentro de Análisis Funcional y Aplicaciones, held in Salobreña (Granada), Spain, 2008. Talk by C. Palazuelos, joint work with C. Fernández-González and D. Pérez-García.

Measurements incompatible in quantum theory cannot be measured jointly in any other no-signaling theory, presented in the 13th Workshop on Quantum Information Processing, QIP2010, held in Zürich, Switzerland, 2010. Talk by M. M. Wolf, joint work with D. Pérez-García and C. Fernández-González.

Sistemas cuánticos: límite termodinámico y operadores no acotados, presented in the conference VII Encuentro de Análisis Funcional y Aplicaciones, held in Jaca (Huesca), Spain, 2011. Talk by C. Fernández-González, joint work with N. Schuch, M. M. Wolf, J. I. Cirac and D. Pérez-García.

Gapless Hamiltonians for non-injective Matrix Product States, presented in the workshop Networking tensor networks: many-body systems and simulations , held in Benasque (Huesca), Spain, 2012. Talk by C. Fernández-González, joint work with N. Schuch, M. M. Wolf, J. I. Cirac and D. Pérez-García.

Gapless Hamiltonians for non-injective PEPS, presented in the Benasque Symposium on Topological Quantum Information, held in Benasque (Huesca), Spain, 2012. Talk by C. Fernández-González, joint work with N. Schuch, M. M. Wolf, J. I. Cirac and D. Pérez-García.

Poster presentations:

Gapless Hamiltonians for the toric code using the PEPS formalism, presented in the 16th Workshop on Quantum Information Processing, QIP2013, held in Beijing, China, 2013. Work by C. Fernández-González, N. Schuch, M. M. Wolf, J. I. Cirac and D. Pérez-García.

CHAPTER 2

Introduction to the quantum formalism.

Quantum Mechanics formalism is based on four postulates on which the whole theory stems, described in the language of Hilbert spaces. Let us introduce them in this chapter, together with some basic concepts we will need throughout this work. All these contents can be found, for instance, in [**91**].

The first postulate states how properties of matter, or states, are described within a single system.

POSTULATE 2.1. *Associated to any isolated system, there is a complex Hilbert space known as the space of the system. The system at a given moment is described by the state of the system, which is a unitary vector from the Hilbert space of the system.*

Dirac notation will be used very often, mainly in chapters 4, 5 and 6. Vectors will be denoted by kets – $|\cdot\rangle$ –, and their duals will be denoted by bras – $\langle\cdot|$. The scalar product of two vectors $|\varphi\rangle$ and $|\psi\rangle$ will be denoted as $\langle\varphi|\psi\rangle$, being therefore the second entry the linear one.

With this notation we will also use rank-one operators in a system A with the form

$$\begin{array}{rccc} |\psi\rangle\langle\varphi|: & A & \longrightarrow & A \\ & |\eta\rangle & \mapsto & \langle\varphi|\eta\rangle|\psi\rangle \end{array}$$

Note that, for normalized states, $|\varphi\rangle\langle\varphi|$ is the projector onto the linear space spanned by $|\varphi\rangle$.

We will usually identify the systems with their associated Hilbert spaces, which can be infinite dimensional – e.g., when describing the position of a particle – or finite dimensional – e.g., when considering spins. The canonical basis elements of an n-dimensional Hilbert space will be often denoted by the vectors

$$|0\rangle,\ |1\rangle, \dots,\ |n-1\rangle.$$

When the Hilbert space has dimension two, vectors are sometimes called qubits, in analogy to the bits 0 and 1 which are used in classical information settings. If the space has dimension d vectors may be called qudits.

Therefore, typical states expressed in terms of these basis elements would be

$$a|0\rangle + b|1\rangle,\ \text{with } a, b \in \mathbb{C} \text{ and } |a|^2 + |b|^2 = 1,\ \text{and}$$

$$a_0|0\rangle + a_1|1\rangle + \cdots + a_{n-1}|n-1\rangle,\ \text{with } a_i \in \mathbb{C} \text{ and } \sum_{i=0}^{n-1} |a_i|^2 = 1.$$

Such configurations, when a and b are both nonzero or at least two scalars in the second expression are nonzero, are sometimes called superpositions of the different basis elements. In oposition to classical information in which bits can be only 0 or 1, in quantum information we can 'have both' 0 and 1 with different possible weights. The same difference arises when considering longer bit strings. Linear combinations of arbitrary vectors not coming from a basis will also be sometimes called superpositions.

Two of such superpositions are the states

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \text{ and } |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}},$$

which form an orthonormal basis of $\mathbb{C}^2$ and which we will also use.

Additionally, in order to make expressions clearer and so as not te be writing continuously the norm, we will also consider unnormalized vectors as unnormalized states. Whenever this distinction is relevant – e.g., when calculating energies of states – we will pay special attention and will calculate and take into account the norms of the involved states.

The second postulate describes how different systems are described when put together and considered as a unique system.

POSTULATE 2.2. *Given two systems A and B, the composite system is associated to the Hilbert space $A \otimes B$. Given $|\varphi_1\rangle \in A$ and $|\varphi_2\rangle \in B$ describing the states of these systems, the composite state is described in the composite system as $|\varphi_1\rangle \otimes |\varphi_2\rangle \in A \otimes B$.*

The composite system described by two vectors as $|\varphi_1\rangle \otimes |\varphi_2\rangle$ will often be denoted as $|\varphi_1\varphi_2\rangle$. For n different systems, respectively in states $|\varphi_i\rangle$, $i = 1, \dots, n$, we would have the composite state

$$|\varphi_1\rangle \otimes |\varphi_2\rangle \otimes \cdots \otimes |\varphi_n\rangle = |\varphi_1\varphi_2\cdots\varphi_n\rangle.$$

A and B are called subsystems of the composite system $A \otimes B$.

Note that not every element of the composite system has such product description, since superpositions are also allowed in this composite system. For example, states as $(|00\rangle + |11\rangle)/\sqrt{2}$ are also in the composite system even though they might not come from two individual states in the subsystems. This will be very important, as we will comment later when introducing entanglement.

The third postulate describes how systems can evolve.

POSTULATE 2.3. *The evolution from an instant t_1 to an instant t_2 of an isolated physical system A is always given by a unitary operator*

$$U_{t_1,t_2} : A \to A$$

And, finally, the fourth postulate states how we can get information from the quantum states, i.e., how we can perform measurements on the systems.

POSTULATE 2.4. *Given a set $\{\Pi_i\}_{i\in I}$, $I \subset \mathbb{R}$, of mutually orthogonal projections in a Hilbert space A which sum up to the identity, and given a state $|\varphi\rangle \in A$, we can perform a measurement – called projective measurement – on the state using the projections $\{\Pi_i\}_{i\in I}$. The possible outcomes of the measurement are the different labels i of the set of projections,* *the probability of getting outcome i is $\langle\varphi|\Pi_i|\varphi\rangle$, and in this case the state will end up transformed after the measurement in the state $\Pi_i|\varphi\rangle/\|\Pi_i|\varphi\rangle\|$.*

If we perform the measurement corresponding to the projectors $\Pi_0 = |0\rangle\langle 0|$ and $\Pi_1 = |1\rangle\langle 1|$ in a 2-dimensional space on a state $a|0\rangle + b|1\rangle$, we get the outcome 0 with probability $|a|^2$ and the outcome 1 with probability $|b|^2$. Recall that the state needed to be normal, therefore $|a|^2 + |b|^2 = 1$, and the outcome probabilities are a complete probability distribution. This happens for every measurement and every state.

Since every Hermitian operator O on a finite dimensional space can be diagonalized in mutually orthogonal eigenspaces, $O = \sum_{i=1}^{k} \lambda_i \Pi_{\lambda_i}$, $\lambda_i \in \mathbb{R}$, every such operator defines a projective measurement respective to the projectors $\{\Pi_{\lambda_i}\}$ onto the respective eigenspaces. As the probability of getting outcome λ_i when performing this measurement on a state $|\varphi\rangle$ is $\langle\varphi|\Pi_{\lambda_i}|\varphi\rangle = \|\Pi_{\lambda_i}|\varphi\rangle\|^2$, we have that the expectaction value $\langle O\rangle_{|\varphi\rangle}$ in this case is

$$\langle O\rangle_{|\varphi\rangle} = \sum_i \lambda_i \langle\varphi|\Pi_{\lambda_i}|\varphi\rangle = \sum_i \langle\varphi|(\lambda_i \Pi_{\lambda_i})|\varphi\rangle = \langle\varphi|O|\varphi\rangle.$$

Hermitian operators will be called observables when decribing such measurements.

A very important class of observables are Hamiltonians, which are the observables corresponding to the energy of the system. They describe the time evolution of systems as stated by Schrödinger equation:

$$H(t)|\varphi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\varphi(t)\rangle.^1$$

For time-independent Hamiltonians, i.e. $H(t) = H \ \forall t$, we have that the unitary evolution is given by

$$U(t) = e^{\frac{-it}{\hbar}H}, \text{ and } |\varphi(t)\rangle = U(t)|\varphi(0)\rangle.$$

Hamiltonians can also be found as the generators of time-independent unitary evolutions. Such evolutions are represented by one-parameter unitary semigroups $\{U(t)\}_{t\in\mathbb{R}^+}$, so that $t \mapsto U(t)$ is a semigroup homomorphism. Stone's Theorem states that, under an additional non very restrictive condition[2], there exists a unique self-adjoint operator H such that $U(t) = e^{\frac{-it}{\hbar}H}$. Such operator is the Hamiltonian governing the evolution.

Note that two states spanning the same linear space would give the same statistics under any measurement. Hence, for measuring purposes, we can identify all these states in an equivalence class, and also with the projector onto their span. The complex coefficients relating two linearly dependent states are called phases. Therefore, two linearly dependent states can be said to be equal up to a phase.

Having this last statement into account, one can easily check that the eigenvectors of a Hamiltonian are fixed points of the unitary evolution associated to them – only phases

[1] $\hbar$ is Planck's constant, which can sometimes be found incorporated to the Hamiltonian, leaving the unitary evolution as $U(t) = e^{-itH}$ for time-independent Hamiltonians.

[2] In the case the one-parameter semigroup is strongly continuous, i.e. the homomorphism $t \mapsto U(t)$ is continuous in the strong operator topology, and $U_0 = \mathbb{I}$. Note that in finite-dimensional spaces every one-parameter weakly continuous unitary semigroup is strongly continuous. Stone's Theorem can be found, for instance, in **[20]** and **[32]**.

are acquired by these states during such evolution.

We will focus on the eigenvectors corresponding to the lowest energy levels – lowest spectral values – of the Hamiltonians, which capture the physics of the system when the evolution is determined by a given Hamiltonian and is kept under 'low temperature'.

Definition 2.5. Given a lower bounded Hamiltonian H, a state $|\varphi\rangle$ is a ground state of H if $|\varphi\rangle$ is an eigenvector of H for its lowest spectral value. The set of all ground states of a given Hamiltonian is called the ground state space – or simply ground space – of the Hamiltonian.

Hamiltonians on finite-dimensional spaces always have ground states, since the whole spectrum is punctual in this case. We will also work with Hamiltonians in infinite-dimensional spaces, and they all will also have ground state space, since they will be positive operators – therefore bounded from below – with non trivial kernel. We will say that the ground state is unique – up to a phase – if the ground state space is one-dimensional; if the dimension of the ground state space is larger than 1 we will say the Hamiltonian and the ground state space are degenerate.

If we turn now the look to states in composite systems, there arise two very important features: mixed states and entanglement.

Whenever we only have control on one of the subsystems, the projective measurements we can perform have the form $\Pi_i \otimes \mathbb{I}$ – or $\mathbb{I} \otimes \Pi_i$ –, and all the information we can get from a state is that coming from the corresponding reduced density matrix. For this, we need to 'trace out' one of the subsystems.

Definition 2.6. Given two Hilbert spaces A and B, the partial trace with respect to B is the unique linear map

$$\mathrm{tr}_B : L(A \otimes B) \to L(A)$$

such that

$$\mathrm{tr}_B(R \otimes S) = \mathrm{tr}(S)R, \ \forall R \in L(A), \ \forall S \in L(B).$$

Definition 2.7. Given a state $|\varphi\rangle \in A \otimes B$, the reduced density matrix of this state corresponding to the subsystem A is $\mathrm{tr}_B(|\varphi\rangle\langle\varphi|)$.

Operationally, for finite dimensional spaces, given an orthonormal basis $\{|i\rangle\}_{i=1}^{\dim(B)}$ of B and a block-matrix representation $|\varphi\rangle\langle\varphi| = (T_{kl})_{k,l=1}^{\dim(B)}$, with $T_{kl} \in \mathcal{M}_{\dim(A)}$, we would have

$$\mathrm{tr}_B(|\varphi\rangle\langle\varphi|) = \sum_{k=1}^{\dim(B)} T_{kk} \ .$$

Note that this matrix does not depend on the choice of basis from B, but does depend on the choice of basis of A as matrix representations of linear operators do.

Reduced density matrices, also called density operators, can always be expressed as a convex combination of rank-one projectors, and this is why they are also called mixed states – when they do not have rank one –, or sometimes ensembles when trying to specify which projectors they can be decomposed into. The set of all density operators, for a given physical dimension n, is the set of positive matrices $M \in \mathcal{M}_n$ such that $\mathrm{tr}(M) = 1$.

The same mixed state may come from very different ensembles, and from very different pure states. As an example, the mixed state, with equal weights, coming from projectors $|0\rangle\langle 0|$ and $|1\rangle\langle 1|$ is the same as the one coming from $|+\rangle\langle +|$ and $|-\rangle\langle -|$: They are both the matrix $\mathbb{I}/2$. Therefore, if we consider the states $|\varphi_1\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ and $|\varphi_2\rangle = (|+0\rangle + |-1\rangle)/\sqrt{2}$ and we only have control on the first subsystem, we will never be able to distinguish between them. For many tasks, mixed states must be taken into account, regardless to the ensemble they come from.

In opposition to this type of states, states as elements in the Hilbert space of the system – those introduced in Postulate 2.1 – are called pure states. Even though most of the work is related to pure states, we will refer to mixed states at some points. Whenever we call them just states we will be referring to pure states, unless we say 'the state ρ' or similar expression, where the lack of the ket notation already indicates this is a mixed state.

The other important feature in composite systems we are introducing now is entanglement.

DEFINITION 2.8. A state $|\varphi\rangle \in A \otimes B$ is called separable if there exist states $|a\rangle \in A$ and $|b\rangle \in B$ such that $|\varphi\rangle = |a\rangle \otimes |b\rangle$. In other case, the state is called entangled.

If we consider more than two substems, a pure state $|\varphi\rangle \in \otimes_i A_i$ is called separable if there exist states $|a_i\rangle \in A_i$ such that $|\varphi\rangle = \otimes_i |a_i\rangle$.

EXAMPLE 2.9.
$|\varphi_1\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ is entangled. This state is called the EPR[3] state, or EPR pair.

$|\varphi_2\rangle = \frac{|000\rangle + |011\rangle}{\sqrt{2}}$ is not entangled if we consider that the first subsystem corresponds to the first qubit and the second subsystem to the second and third qubits: $|\varphi_2\rangle = |0\rangle \otimes \frac{|00\rangle + |11\rangle}{\sqrt{2}}$. However, $|\varphi_2\rangle$ is entangled if one of the subsystems consists of the first and second qubits and the other corresponds to the third qubit. $|\varphi_2\rangle$ is also entangled if we consider a partition into three different subsystems corresponding to the three qubits.

$|\varphi_3\rangle = \frac{|100\rangle + |010\rangle + |001\rangle}{\sqrt{3}}$ is entangled for any partition we may consider. This state will be called the 3-qubit W state.

This property is crucial in many fundamental questions and applications within Quantum Mechanics: non-local correlations, teleportation, quantum cryptography, etc. Quantification of entanglement is therefore very important for many tasks, thus it has been extensively studied, mainly in the bipartite setting. In this case, in which we consider bipartite systems, the entropy of entanglement – or entanglement entropy – is one of the most used measures of entanglement[4]. For calculating it, we also use the reduced density matrix corresponding to one of the systems, tracing out the other one.

DEFINITION 2.10. Given a state $|\varphi\rangle \in A \otimes B$, we define its entropy of entanglement respective to the partition $A|B$ as the Shannon entropy S of the eigenvalues $\{\lambda_i\}$ of its

[3]Named after Einstein, Podoslky and Rosen.

[4]All useful measures of entanglement in bipartite settings are essentially equivalent [**63**].

reduced density matrix corresponding to any of the subsystems A or B:

$$\rho(|\varphi\rangle) = S(\mathrm{tr}_A(|\varphi\rangle\langle\varphi|)) = S(\mathrm{tr}_B(|\varphi\rangle\langle\varphi|)) = -\sum_i \lambda_i \log(\lambda_i).$$

This value does not depend on the system we choose to trace out when considering the reduced density matrix, since both reduced density matrices corresponding to either A or B have the same eigenvalues, due to the existence of Schmidt decompositions[5] for bipartite states: Given a state $|\varphi\rangle \in A \otimes B$ – let us suppose $\dim(A) \leq \dim(B)$ – there can be found orthonormal bases $\{|i_A\rangle\}_{i=0}^{\dim(A)-1}$ and $\{|i_B\rangle\}_{i=0}^{\dim(B)-1}$ of A and B respectively such that $|\varphi\rangle = \sum_{i=0}^{\dim(A)-1} \alpha_i |i_A i_B\rangle$ for some coefficients α_i. The eigenvalues of both reduced density matrices with respect to either A or B are $\lambda_i = |\alpha_i|^2$.

For product states $|\varphi\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle$, the respective reduced density matrices are $|\varphi_1\rangle\langle\varphi_1|$ and $|\varphi_2\rangle\langle\varphi_2|$, both with rank 1. Therefore, in this case $\rho(|\varphi\rangle) = 0$, whereas for entangled states we always have $\mathrm{rank}(\mathrm{tr}_A(|\varphi\rangle\langle\varphi|)) > 1$ and $\rho(|\varphi\rangle) > 0$.

It is useful to extend the notion of separability to mixed states, whenever they can be expressed as ensembles of separable states.

DEFINITION 2.11. A mixed state ρ is called separable if it can be expressed as a convex combination of rank-one projectors, each of them being a projector onto the span of a separable pure state.

Equivalently, a mixed state ρ is separable if there exists some Hilbert space C, and some states $\{|\varphi_i\rangle\}$ in A, $\{|\psi_i\rangle\}$ in B and $\{|\chi_i\rangle\}$ in C – this last set formed by mutually orthogonal states – such that

$$\rho \propto \mathrm{tr}_{A\otimes B}(\sum_i |\varphi_i \psi_i \chi_i\rangle),$$

where $\propto$ means 'proportional to'. Note that the vector $|\Phi\rangle = |\varphi_i \psi_i \chi_i\rangle$ used in this last equation is not normalized. The state $|\Phi\rangle / \||\Phi\rangle\|$ is called a purification of the mixed state ρ.

The rest of definitions will be introduced in the subsequent chapters, as we need them.

[5] Schmidt decomposition of bipartite states can be obtained easily as a consequence of the singular value decomposition of matrices.

CHAPTER 3

Rearrangement invariant structures in tensor products.

One of the most interesting properties arising from Quantum Mechanics is that some states in composite systems may show an exceptional characteristic called entanglement. Entangled states enable operations at distant places that are not possible within Classical Mechanics, such as quantum teleportation or quantum cryptography. Two states have the same type of entanglement if they can be mutually transformed by only using local unitary operations (LU), but the point of view of entanglement as a resource motivated an ordering, in which local measurement operations and classical communication are allowed (LOCC). If a given a state $|\varphi\rangle$ can be converted in this LOCC setting into another state $|\psi\rangle$ the first one is more resourceful than the second. This is denoted by

$$|\varphi\rangle \to |\psi\rangle, \text{ or } |\varphi\rangle \overset{\text{LOCC}}{\longrightarrow} |\psi\rangle.$$

In the pure state bipartite setting, it was proved [**78**] that one round of one-way communication is enough, and LOCC convertibility has been characterized [**90**] in terms of the majorization of the eigenvalues of the reduced density matrices, $\bar{\lambda}_{|\varphi\rangle} = (\lambda_1, \dots, \lambda_n)$ and $\bar{\mu}_{|\psi\rangle} = (\mu_1, \dots, \mu_n)$,

$$|\varphi\rangle \to |\psi\rangle \iff \sum_{i=1}^{k} \lambda_i^* \leq \sum_{i=1}^{k} \mu_i^*, \ k = 1, \dots, n$$

where $\bar{\lambda}^*_{|\varphi\rangle}$ and $\bar{\mu}^*_{|\psi\rangle}$ are the respective decreasing rearrangements of $\bar{\lambda}_{|\varphi\rangle}$ and $\bar{\mu}_{|\psi\rangle}$. LU equivalence is characterized by $\bar{\lambda}^*_{|\varphi\rangle} = \bar{\mu}^*_{|\psi\rangle}$.

The possibility of using, in some cases, a catalysist for performing such operation [**64**], i.e. the existence of states $|\varphi\rangle$, $|\psi\rangle$ and $|c\rangle$ such that

$$|\varphi\rangle \not\to |\psi\rangle, \text{ and } |c\rangle \otimes |\varphi\rangle \to |c\rangle \otimes |\psi\rangle;$$

and the existence of states $|\varphi\rangle$ and $|\psi\rangle$ not related by LOCC but such that $\otimes^n|\varphi\rangle$ and $\otimes^n|\psi\rangle$ are [**14**], motivated two related orderings, respectively called ELOCC – for entanglement assisted LOCC – and MLOCC – for multiple-copy LOCC. These orderings were characterized by Aubrun and Nechita in terms of p-norms [**10**]: $|\varphi\rangle$ can be almost converted into $|\psi\rangle$ by either MLOCC or ELOCC iff $\|\bar{\lambda}_{|\varphi\rangle}\|_p \geq \|\bar{\mu}_{|\psi\rangle}\|_p$ $\forall p \geq 1$, where the 'almost' comes from the need of considering in some cases infinite dimensional catalysts.

The characterization of LU equivalence – $\lambda^* = \mu^*$ – makes clear that any characterization of these settings must involve rearrangement invariant properties, and ELOCC and MLOCC settings evidence that they also need some multiplicative properties. With that in hand, we wondered whether symmetry and multiplicativy are the only conditons for finding Aubrun and Nechita's characterization, leading to the first problem we tackle:

> Given two spaces X and Y with symmetric bases, when is the product basis in $X\hat{\otimes}_\alpha Y$ a symmetric basis for some crossnorm α?

We also pose the equivalent problem in continuous rearrangement invariant spaces, for $\Omega = [0,1], \mathbb{R}^+$:

> Given two r.i. spaces $X(\Omega_1)$ and $Y(\Omega_2)$, in which cases do we have
> $$X(\Omega_1)\hat{\otimes}_\alpha Y(\Omega_2) = Z(\Omega_1 \times \Omega_2)$$
> for some r.i. space Z and some crossnorm α?

The first question leads us exactly to Aubrun and Nechita's condition, $X = Y = \ell_p$ and $\alpha = \Delta_p$, plus the case $X = Y = c_0$ and $\alpha = \varepsilon$, the injective crossnorm.

We also solve the second question with an almost analogue answer: $X = Y = Z = L_p$ and $\alpha = \Delta_p$.

3.1. Symmetric structures on tensor products of spaces with bases.

We first introduce the basic definitions we need for this section, starting with symmetric and subsymmetric bases.

Definition 3.1.1. Let X be a separable Banach space with Schauder basis
$$B = (x_n)_{n=1}^\infty \subset X.$$
The basis is called symmetric if for every permutation $\pi : \mathbb{N} \to \mathbb{N}$ the basis $\{x_{\pi(n)}\}_{n=1}^\infty$ is equivalent to $\{x_n\}_{n=1}^\infty$.

A positive constant K, the symmetric basis constant of B, can be found as the supremum of the norms of these equivalences. The space can be given an equivalent norm so that the symmetric constant of this basis turns to be one.

Definition 3.1.2. Let X be a separable Banach space with Schauder basis
$$B = (x_n)_{n=1}^\infty \subset X.$$
The basis is called subsymmetric if every subsequence $(x_{n_k})_{k=1}^\infty$ is a basic sequence equivalent to the basis.

It turns out that every symmetric basis is also subsymmetric. Moreover, if a symmetric basis constant is K for a given symmetric basis, its subsequences are K-equivalent to it.

We will also need a few notions about tensor products and crossnorms. An extensive picture of crossnorms can be found in [**34**]. Given two Banach spaces X and Y, we say that α is a reasonable crossnorm whenever it satisfies the conditions:

(1) $\alpha(x \otimes y) \leq \|x\|\|y\|$ for all $x \in X$ and $y \in Y$, and
(2) if $x^* \in X^*$ and $y^* \in Y^*$, then $x^* \otimes y^* \in (X \otimes Y, \alpha)^*$ and its functional norm is upper bounded by $\|x^*\|\|y^*\|$.

In what follows, we will simply refer to a reasonable crossnorm as a crossnorm. It is very easy to check that, actually, both inequalities are equalities.

There are two particularly interesting crossnorms on the tensor product $X \otimes Y$. The projective crossnorm, defined by
$$\pi(u) = \inf\{\sum_{i=1}^n \|x_i\|\|y_i\|\},$$

where the infimum is taken over all the representations of $u = \sum_{i=1}^n x_i \otimes y_i \in X \otimes Y$. And the injective crossnorm, defined by

$$\varepsilon(u) = \sup\{|\langle u, x^* \otimes y^* \rangle| : x^* \in B_{X^*}, y^* \in B_{Y^*}\}.$$

Here B_{X^*} denotes the closed unit ball of the dual space X^* of X ,and the same for Y. It follows easily that every crossnorm α satisfies $\varepsilon \leq \alpha \leq \pi$.

We need to define a family of crossnorms which will be crucial in our results. Let (Ω, μ) be an arbitrary measure space and E a normed space. Then, following [**34**], Sec. 7, for any $p \in [1, \infty)$ we consider the spaces of – classes of a.e. equal – Bochner p-Integrable functions $\Omega \longrightarrow \hat{E}$, $L_p(\mu, \hat{E})$, where $\hat{E}$ is the completation of E . If we consider the injective natural mapping

$$L_p(\mu) \otimes E \hookrightarrow L_p(\mu, \hat{E}) \tag{1}$$

defined by $\tilde{f} \otimes x \mapsto \tilde{f}(\cdot)x$, we can define the crossnorm

$$\Delta_p(f; L_p, E) := \Big(\int_\Omega \|f(w)\|_E^p d\mu(w) \Big)^{\frac{1}{p}} \tag{2}$$

on $L_p \otimes E$. We denote the corresponding normed space by $L_p \otimes_{\Delta_p} E$ and by $L_p \hat{\otimes}_{\Delta_p} E$ its completion. It is not difficult to see that $\Delta_1 = \pi$ on $L_1 \otimes E$ and, using a density argument with the simple functions, it follows that $L_p \hat{\otimes}_{\Delta_p} E$ and $L_p(\mu, \hat{E})$ are isometrically isomorphic. In particular, given two arbitrary measure spaces (Ω_1, μ_1) and (Ω_2, μ_2), for every $1 \leq p < \infty$ we have the isometric identifications

$$L_p(\mu_1 \otimes \mu_2) = L_p(\mu_1) \hat{\otimes}_{\Delta_p} L_p(\mu_2) = L_p(\mu_1, L_p(\mu_2)). \tag{3}$$

Recall that separable spaces with bases can be considered as measure spaces on $\mathbb{N}$ with the discrete measure. In this case we will omit, as it is usually done, the measure space when referring to the well-known spaces ℓ_p.

The question would then be: which Banach spaces X and Y with symmetric bases and which crossnorms α can be put together so that the product basis is a symmetric basis of the tensor product $X \hat{\otimes}_\alpha Y$?

Let X and Y be Banach spaces with symmetric bases $\{x_n\}_{n=1}^\infty$ and $\{y_n\}_{n=1}^\infty$ respectively, and let α be a crossnorm. The product basis in $Z = X \hat{\otimes}_\alpha Y$ is $\{x_n \otimes y_m\}_{n,m=1}^\infty$, together with certain order – see [**77**] – which makes $\{x_n \otimes y_1\}_{n=1}^\infty$ and $\{x_1 \otimes y_m\}_{m=1}^\infty$ subsequences of the product basis sequence.

Remark 3.1.3. With the simple previous property that every symmetric basis is also subsymetric we can establish that the spaces X, Y and Z must be necessarily the same. If the product basis is a symmetric basis of the tensor product then $\{x_n \otimes y_1\}_{n=1}^\infty$, $\{x_1 \otimes y_n\}_{n=1}^\infty$ are subsequences of $\{x_n \otimes y_m\}_{n,m=1}^\infty$, and they are all equivalent. Since the sequence $\{x_n \otimes y_1\}_{n=1}^\infty$ is equivalent to $\{x_n\}_{n=1}^\infty$ and $\{x_1 \otimes y_n\}_{n=1}^\infty$ is equivalent to $\{y_n\}_{n=1}^\infty$ we have that X, Y and Z are the same space.

We will also need the following characterization of the spaces ℓ_p and c_0 from [**3**]: there must exist a constant $K > 0$ such that

$$K^{-1}\|a\| \cdot \|b\| \leq \| \sum_{i,j=1}^\infty a_i b_j e_{i,j} \| \leq K \|a\| \cdot \|b\|$$

for all vectors $a = \sum_{i=1}^{\infty} a_i e_i$, $b = \sum_{i=1}^{\infty} b_j e_j$ in the space, and $\{e_{i,j}\}_{j=1}^{\infty}$, $i \in \mathbb{N}$ disjoint subsequences of the product basis.

We have now all the tools we need to prove the main result of this section.

THEOREM 3.1.4. *If X, Y are spaces with symmetric bases $\{x_n\}_{n=1}^{\infty}$ and $\{y_n\}_{n=1}^{\infty}$ respectively, such that there exists a crossnorm α that makes $\{x_n \otimes y_m\}_{n,m=1}^{\infty}$ a symmetric basis in $Z = X\hat{\otimes}_\alpha Y$, then $X = Y = Z$ is the space ℓ_p and $\alpha = \Delta_p$ for some $1 \le p < \infty$, or it is the space c_0 and $\alpha = \varepsilon$.*

PROOF. Let us rename the symmetric basis in the tensor product just with one index: $\{x_n \otimes y_m\}_{n,m=1} = \{e_k\}_{k=1}^{\infty}$, for certain bijection $\pi : \mathbb{N}\times\mathbb{N} \to \mathbb{N}$. Let C be its symmetric constant.

Let $a = \sum_i a_i e_i$ and $b = \sum_i b_i e_i$ be vectors in Z, and $\{e_{k,l}\}_{l=1}^{\infty}, k \in \mathbb{N}$ a family of disjoint subsequences of the product basis.

We can consider the vector $\sum_{i,j} a_i b_j e_{i,j}$, whose norm can be bounded as

$$C^{-1}\|\sum_{i,j} a_i b_j x_i \otimes y_j\| \le \|\sum_{i,j} a_i b_j e_{i,j}\| \le C\|\sum_{i,j} a_i b_j x_i \otimes y_j\|. \tag{4}$$

Recall that

$$\|\sum_{i,j} a_i b_j x_i \otimes y_j\| = \|\sum_i a_i x_i\|\|\sum_j b_j y_j\| = \frac{\|\sum_i a_i x_i \otimes y_1\|\|\sum_j b_j x_1 \otimes y_j\|}{\|x_1\|\|y_1\|}, \tag{5}$$

and since the product basis is subsymmetric we have the bounds

$$C^{-1}\|a\| \le \|\sum_i a_i x_i \otimes y_1\| \le C\|a\| \tag{6}$$

$$C^{-1}\|b\| \le \|\sum_j b_j x_1 \otimes y_j\| \le C\|b\|. \tag{7}$$

We can then assure

$$\|\sum_{i,j} a_i b_j e_{i,j}\| \le C\|\sum_{i,j} a_i b_j x_i \otimes y_j\| = C\frac{\|\sum_i a_i x_i \otimes y_1\|\|\sum_j b_j x_1 \otimes y_j\|}{\|x_1\|\|y_1\|} \le \frac{C^3\|a\|\|b\|}{\|x_1\|\|y_1\|}$$

and

$$\|\sum_{i,j} a_i b_j e_{i,j}\| \ge \frac{C^{-3}}{\|x_1\|\|y_1\|}\|a\|\|b\|$$

Any value $K \ge \max\left\{\frac{C^3}{\|x_1\|\|y_1\|}, C^3\|x_1\|\|y_1\|\right\}$ would prove that $Z = \ell_p$ or c_0 following the characterization we recalled before. □

As a consequence of this result we can assure that there could not be a Pisier-Schütt type theorem in the context of symmetric bases. This is due to a result by Read [**108**], regarding a space E and the space of doble sequences $E[E]$.

$E[E]$ is defined on the product basis equipped with the norm

$$\beta(\sum_{i,j} a_{i,j} e_i \otimes e_j) = \|\sum_i \|\sum_j a_{i,j} e_j\|_E \; e_i\|_E,$$

which is a crossnorm.

E has a symmetric basis and E and $E[E] = E\hat{\otimes}_\beta E$ are isomorphic. In the case there existed a Pisier-Schütt type theorem for symmetric bases, this would imply that the product basis of $E[E]$ should be also symmetric. And, following our preceeding result, this would imply that E should be either c_0 or some ℓ_p, $1 \le p < \infty$, which is not the case.

The universal space for unconditional bases U_1 Pełczyński found in [**99**] could also serve as a counterexample, together with the same crossnorm β.

3.2. Rearrangement invariant structures on tensor products of rearrangement invariant spaces.

In this section we consider an equivalent question regarding rearrangement invariant (r.i.) spaces. We start with some definitions we will need. We refer to [**77**] for a complete work on r.i. theory.

Let $(\Omega, \Sigma, \lambda)$ be a measure space. We also consider the product measure space denoted by $(\Omega \times \Omega, \Sigma \otimes \Sigma, \lambda \times \lambda)$.

We denote by $\mathcal{M}_0(\Omega)$ (resp. $\mathcal{M}_0(\Omega \times \Omega)$) the set of measurable functions on Ω (resp. on $\Omega \times \Omega$) over $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$.

Definitions 3.2.1. Given a function $f \in \mathcal{M}_0(\Omega)$,

(1) we denote by μ_f the distribution function of f, defined as
$$\mu_f(x) := \lambda\{t \in \Omega : |f(t)| > x\},$$
for every $x \ge 0$,

(2) we will say that two measurable functions f, g on Ω are equimeasurable if they have the same distribution function,

(3) we denote by f^* the decreasing rearrangement of f, defined as
$$f^*(t) := \inf\{x : \mu_f(x) \le t\}, \ t \in [0, \infty).$$

Definition 3.2.2. A Banach function space X on Ω is said to be a rearrangement invariant space if the next property holds:

If we have $f, g \in \mathcal{M}_0(\Omega)$ such that $f^*(t) \le g^*(t)$ for every $t \in [0, \infty)$ and $g \in X(\Omega)$, then $f \in X(\Omega)$ and $\|f\|_X \le \|g\|_X$.

It follows that if $X(\Omega)$ is an r.i. space on Ω and $f, g \in \mathcal{M}_0(\Omega)$ are equimeasurable, then $f \in X(\Omega) \Leftrightarrow g \in X(\Omega)$ and, in this case, $\|f\|_X = \|g\|_X$.

Following [**77**], 2.a, we will consider $(\Omega, \Sigma, \lambda)$ a separable measure space. This implies that the study of the r.i. spaces over $(\Omega, \Sigma, \lambda)$ reduces immediately to the cases $\Omega = I = [0,1]$ with the usual Lebesgue measure λ, $\Omega = [0, \infty)$ with the usual Lebesgue measure λ, and the case in which Ω is the set of integers with the discrete measure. We already studied this last case for Banach spaces with symmetric basis.

When we have an r.i. space $X = X(\Omega)$ on Ω, the corresponding r.i. space $X(\Omega \times \Omega)$ on $\Omega \times \Omega$ is the space of measurable functions $x(s,t)$ on $\Omega \times \Omega$ such that $x^*(t) \in X(\Omega)$, with the norm $\|x\|_{X(\Omega\times\Omega)} = \|x^*\|_{X(\Omega)}$, where x^* denotes the decreasing rearrangement of

x.

To agree with the results of [**9**] and [**62**], which we will use, we assume that every r.i. X is either separable or it has the Fatou property.

We will need to use that for every r.i. space $X(I)$ we have continuous embeddings

$$L_\infty(I) \hookrightarrow X(I) \hookrightarrow L_1(I),$$

both with norm equal to one. And for every r.i. space $Y(0,\infty)$ we have continuous embeddings

$$L_\infty(0,\infty) \cap L_1(0,\infty) \hookrightarrow Y(I) \hookrightarrow L_\infty(0,\infty) + L_1(0,\infty)$$

also with norm one, and where the norms considered are $\max(\|f\|_1, \|f\|_\infty)$ and $\int_0^1 f^*(t)dt$ in the first and third spaces respectively – see [**77**] 2.a. It follows that we have $\mathcal{S} \subset X(\Omega)$, where $\mathcal{S}$ denotes the set of simple functions on Ω.

We will also use the family of crossnorms defined in eq. (2) from previous section, and the $L_p(\Omega)$ measure spaces. In the case $p = \infty$, for a normed space E, with completion $\hat{E}$, $L_\infty(\mu, \hat{E})$ is the space of – classes of locally a.e. equal – bounded μ-measurable functions $\Omega \longrightarrow \hat{E}$. With the same natural mapping from equation (1) we define now

$$\Delta_\infty(f; L_\infty, E) := \text{ess-sup}\|f(\cdot)\|_E.$$

It is easy to see that $\Delta_\infty = \varepsilon$ on $L_\infty \otimes E$.

Remark 3.2.3. We have to notice here that the isometric identification from eq. (3) is not onto in the case $p = \infty$. It is well known that $L_\infty(\Omega)\hat{\otimes}_\varepsilon L_\infty(\Omega) \subsetneq L_\infty(\Omega \times \Omega)$ in the cases we are considering.

In this section we want to characterize which r.i. Banach spaces X, Y and Z verify that there exists a crossnorm α such that the operator

$$B : X(\Omega) \otimes_\alpha Y(\Omega) \longrightarrow Z(\Omega \times \Omega),$$

defined as $B(x \otimes y)(s,t) = x(s)y(t)$ for every $(s,t) \in \Omega \times \Omega$, is an onto topological isomorphism $\hat{B}$ when we extend it to the completion $X(\Omega)\hat{\otimes}_\alpha Y(\Omega)$.

From the definition of the crossnorms Δ_p, it is obvious that when we consider $X = Y = L_p$ and $\alpha = \Delta_p$ for $1 \le p < \infty$, the statement holds. We want to prove that the converse is also true.

The two cases of Ω we are treating in this section ($\Omega = I = [0,1]$ and $\Omega = [0,\infty)$) admit almost the same proof, so we will show the first one, and we will indicate the slight modifications required in the case $[0,\infty)$.

The next easy remark will be used in the work and it will facilitate some proofs.

Remark 3.2.4. Suppose we have that the operator $\hat{B}$ is a topological isomorphism from $X(I)\hat{\otimes}_\alpha X(I)$ onto $Z(I \times I)$, so B is. Since Z is an r.i. space, it is easy to see that the mapping $j : f \to f \cdot \mathbb{1}$ from $Z(I)$ into $Z(I \times I)$ is a linear isometry onto its image (where $\mathbb{1}$ denotes the characteristic function on I). Then, if we call $i : X(I) \hookrightarrow X(I) \otimes_\alpha X(I)$, defined as $i(f) = f \longrightarrow f \otimes \mathbb{1}$, the application $j^{-1} \circ B \circ i$ is exactly the identity $id : X(I) \hookrightarrow Z(I)$.

Which is then a topological isomorphism (not necessarily onto), with the same norm as B.

Before proving the result we need the following lemma:

LEMMA 3.2.5. *There is not any r.i. space Z and crossnorm α such that the operator $\hat{B}$ is an onto topological isomorphism from $L_\infty(I)\hat{\otimes}_\alpha L_\infty(I)$ onto $Z(I \times I)$.*

PROOF. If $\hat{B} : L_\infty(I)\hat{\otimes}_\alpha L_\infty(I) \longrightarrow Z(I \times I)$ is a topological isomorphism, from Remark 3.2.4 we know that $id : L_\infty(I) \hookrightarrow Z(I)$ is a topological isomorphism. By the definition of $Z(I \times I)$, we have that $id : L_\infty(I \times I) \hookrightarrow Z(I \times I)$ is a topological isomorphism too.

Given an element $a \in L_\infty(I) \otimes L_\infty(I)$, we have

$$\|a\|_{L_\infty(I)\otimes_\alpha L_\infty(I)} \sim \|B(a)\|_{Z(I\times I)} \sim \|B(a)\|_{L_\infty(I\times I)} = \|a\|_{L_\infty(I)\otimes_\varepsilon L_\infty(I)},$$

where $\sim$ denotes equivalence between the norms.

This says that $\alpha \sim \varepsilon$ on $L_\infty(I) \otimes L_\infty(I)$, and thus the completion is the same for both crossnorms. Remark 3.2.3 completes the proof. $\square$

REMARK 3.2.6. The proof above does not depend on the cases of Ω that we are considering.

Following **[9]**, given an r.i. space X on I, we take

$$V_0(X) = \{a \in X : a \neq 0, a = a^*\}.$$

Now, for any function $a \in V_0(X)$ and dyadic intervals $\Delta_{n,k} = [\frac{k-1}{2^n}, \frac{k}{2^n}], k = 1, 2, \cdots, 2^n, n \in \mathbb{N}$, we consider the dilations and translations of the function a:

$$a_{n,k} = \begin{cases} a(2^n t - k + 1) & \text{if } t \in [\frac{k-1}{2^n}, \frac{k}{2^n}], \\ 0 & \text{otherwise.} \end{cases}$$

It follows then that the support of $a_{n,k}$ is contained in $\Delta_{n,k}$, and for every $x > 0$ we have

$$\lambda(\{t \in \Delta_{n,k} : |a_{n,k}(t)| > x\}) = \frac{1}{2^n}\lambda(\{t \in I : |a(t)| > x\}). \tag{8}$$

The key of the proof of our main result is the next result from **[9]**.

THEOREM 3.2.7. **[9]***(Theorem 7) Let X be an r.i. space on $[0,1]$. Then, there exists a $p \in [1,\infty]$ such that $X = L_p$ if and only if there exists a constant $C > 0$ such that*

$$C^{-1}\|\sum_{k=1}^{2^n} c_{n,k}\chi_{\Delta n,k}\|_X\|a\|_X \le \|\sum_{k=1}^{2^n} c_{n,k}a_{n,k}\|_X \le C\|\sum_{k=1}^{2^n} c_{n,k}\chi_{\Delta_{n,k}}\|_X\|a\|_X, \tag{9}$$

for all $a \in V_0(X)$ and all $c_{n,k} \in \mathbb{R}$ with $k = 1, 2, \cdots, 2^n, n = 0, 1, 2, \cdots$.

With this at hand we can prove the next proposition:

PROPOSITION 3.2.8. *Given X, Y and Z r.i. spaces and α a crossnorm, if the operator B is a topological isomorphism from $X(I) \otimes_\alpha Y(I)$ into $Z(I \times I)$, then there must exist a $p \in [1,\infty]$ such that $X = L_p = Y$.*

PROOF. Using that B is a topological isomorphism, we have that there exists a constant M such that for every $x \in X(I) \otimes Y(I)$ it holds that

$$M^{-1}\alpha(x) \leq \| B(x) \|_{Z(I\times I)} \leq M\alpha(x).$$

We have mentioned (see Remark 3.2.4) that $id : X(I) \hookrightarrow Z(I)$ is a topological isomorphism with the same constant M as B (and the same holds for Y). We want to remark the next fact, that we will use later:

If we consider the set of simple functions $\mathcal{S}$ on I, we have that $\mathcal{S} \subset X(I) \cap Y(I) \subset Z(I)$ and, by the comments above, the norms $\|\cdot\|_X$ and $\|\cdot\|_Y$ are equivalent on $\mathcal{S}$ with constant M^2 – in particular, for every $s \in \mathcal{S}$, $\|s\|_Y \leq M^2\|s\|_X$.

Suppose there is no $p \in [1,\infty]$ such that $X = L_p$; we want to reach a contradiction. At least one of the inequalities in (9) must fail. We assume the inequality on the right fails (the reasoning in the other case is analogous). Then, there exists a function $a \in V_0(X)$, a natural number $n \in \mathbb{N}$ and some coefficients $c_{n,k} \in \mathbb{R}$ with $k = 1, 2, \cdots, 2^n$, such that

$$\|\sum_{k=1}^{2^n} c_{n,k}a_{n,k}\|_X > M^4 \|\sum_{k=1}^{2^n} c_{n,k}\chi_{\Delta n,k}\|_X \|a\|_X.$$

We consider the next two elementary tensors in $X(I) \otimes Y(I)$:
$x = \sum_{k=1}^{2^n} c_{n,k}a_{n,k} \otimes \mathbb{1}$, and $y = a \otimes \sum_{k=1}^{2^n} c_{n,k}\chi_{\Delta_{n,k}}$.

We are going to show that $\mu_f = \mu_g$ on $Z(I \times I)$, where $f = B(x)$ and $g = B(y)$. Then, using that Z is an r.i. space, we will have that $\| B(x) \|_{Z(I\times I)} = \| B(y) \|_{Z(I\times I)}$, and thus $\alpha(x) \leq M^2\alpha(y)$. This will be a contradiction because we have chosen the elements x and y such that

$$\alpha(x) = \| \sum_{k=1}^{2^n} c_{n,k}a_{n,k} \|_X \|\mathbb{1}\|_Y = \| \sum_{k=1}^{2^n} c_{n,k}a_{n,k} \|_X >$$

$$> M^4\|a\|_X \|\sum_{k=1}^{2^n} c_{n,k}\chi_{\Delta n,k}\|_X \geq M^2\|a\|_X \|\sum_{k=1}^{2^n} c_{n,k}\chi_{\Delta n,k}\|_Y = M^2\alpha(y).$$

where in the last inequality we have used the inequality described before for simple functions on $X \cap Y$.

Let us prove it. Let $w > 0$. On the one hand we have tht

$$\mu_f(w) = \lambda\{(s,t) \in I \times I : |\sum_{k=1}^{2^n} c_{n,k}a_{n,k}(s)\mathbb{1}(t)| > w\}$$

$$= \lambda\{s \in I : |\sum_{k=1}^{2^n} c_{n,k}a_{n,k}(s)| > w\} = \sum_{k=1}^{2^n} \lambda\{s \in \Delta_{n,k} : |a_{n,k}(s)| > \frac{w}{|c_{n,k}|}\}$$

$$= \frac{1}{2^n}\sum_{k=1}^{2^n} \lambda\{s \in I : |a(s)| > \frac{w}{|c_{n,k}|}\}.$$

We have used (8) in the last step.

On the other hand,

$$\mu_g(w) = \lambda\{(s,t) \in I \times I : |\sum_{k=1}^{2^n} c_{n,k}a(s)\chi_{\Delta_{n,k}}(t)| > w\}$$

$$= \sum_{k=1}^{2^n} \lambda\{(s,t) \in \Delta_{n,k} \times I : |c_{n,k}a(s)| > w\}$$

$$= \sum_{k=1}^{2^n} \lambda(\Delta_{n,k})\lambda\{s \in I : |a(s)| > \frac{w}{|c_{n,k}|}\} = \frac{1}{2^n}\sum_{k=1}^{2^n} \lambda\{s \in I : |a(s)| > \frac{w}{|c_{n,k}|}\}.$$

Hence there must be a $p \in [1,\infty]$ such that $X = L_p$. Similarly we can proceed for Y, and get that there must be a $q \in [1,\infty]$ with $Y = L_q$. And, since $\mathcal{S}$ is dense in both $X(I)$ and $Y(I)$ and the norms are equivalent on the elements of $\mathcal{S}$, we can conclude that $p = q$ and $X = Y$.

□

With this last property and some density arguments we can prove the main result:

THEOREM 3.2.9. *Given X, Y, Z r.i. spaces. Then the operator $\hat{B}$ is a topological isomorphism from $X(\Omega)\hat{\otimes}_\alpha Y(\Omega)$ onto $Z(\Omega \times \Omega)$ if and only if there exists a $p \in [1,\infty)$ such that $X = Y = Z = L_p$ and $\alpha = \Delta_p$.*

PROOF. (Case $\Omega = [0,1]$.)
One of the implications is trivial, let us proceed with the other one.

From the previous theorem we already know that necessarily there exists a $p \in [1,\infty]$ such that $X = L_p(I) = Y$. Now, using lemma 3.2.5 we can rule out the case $X = Y = L_\infty(I)$.

The set S of simple functions on I is dense in $L_p(I)$, and for every crossnorm α, the set $S \otimes S$ is dense in $L_p(I) \otimes_\alpha L_p(I)$, and hence so is $B(S \otimes S)$ in $Z(I \times I)$. Also, we have that $B(S \otimes S)$ is dense in $L_p(I \times I) = L_p(I)\hat{\otimes}_{\Delta_p} L_p(I)$ and, again considering Remark 3.2.4, this space is isomorphically embedded – by the identity – into $Z(I \times I)$. Hence, it is dense in $Z(I \times I)$. Therefore Z must be also L_p and the norm α must be equivalent to the norm Δ_p just by the definition of this crossnorm.

□

The proof of the case $\Omega = [0,\infty)$ can be done following the same steps using Theorem 5.4 from [**62**]. We must mention that in this theorem they need to add the hypothesis $\phi_E(0+) = \phi_{E'}(0+) = 0$. However, we only need to use the equivalence between (ii) and (iv), which also holds without this hypothesis.

We follow the same notation as in [**62**]. Given an r.i. space X on $[0,\infty)$, we take

$$V(X) = \{a \in X : a \neq 0, \operatorname{supp} a \subseteq [0,1), \, a = a^*\}.$$

Then, fixed an element $a \in V(X)$, we consider the translation of $a(t)$ to the interval $[k-1,k)$ for every $k \geq 1$, i.e.

$$a_k(t) = \begin{cases} a(t-(k-1)) & \text{if } t \in [k-1,k), \\ 0 & \text{otherwise.} \end{cases} \qquad \text{for every } k \geq 1.$$

Then, we have the following.

THEOREM 3.2.10. [**62**]*(Theorem 5.4) Let X be an r.i. space on $[0,\infty)$. Then, there exists a $p \in [1,\infty]$ such that $X = L_p$ if and only if there exists a constant $C > 0$ such that*

$$C^{-1}\|\sum_{k=1}^{n} c_k\chi_{[k-1,k)}\|_X\|a\|_X \leq \|\sum_{k=1}^{n} c_k a_k\|_X \leq C\|\sum_{k=1}^{n} c_k\chi_{[k-1,k)}\|_X\|a\|_X, \tag{10}$$

for every natural $n \in \mathbb{N}$, every $a \in V(X)$ and all c_k with $k = 1,2,\cdots$.

This result let us finish the proof of our last theorem.

PROOF. (Theorem 3.2.9, case $\Omega = [0,\infty)$.) We only prove the left to right implication. The other is easy.

Following exactly the same way as in [**62**] (Theorem 5.4), from (10) it follows that the fundamental function of X verifies $\phi_X(t) \approx t^\alpha$ for some $\alpha \in [0,1]$ – we do not rule out the case $\alpha = 0$ in [**62**] (Theorem 5.2). If we are in the case $\alpha \in (0,1)$, we continue the proof as in [**62**] and we get $X = L_p$ for some $p \in (1,\infty)$. For $\alpha = 0,1$ it is known that the only spaces with these fundamental functions are L_1 and L_∞. Note that the space $\Gamma = \overline{S}^{\|\cdot\|_\infty}$, which is the only space besides L_∞ which corresponds to $\alpha = 0$, is not considered since it is not separable and does not have the Fatou property. $\square$

The case $\Omega = [0,\infty)$ follows now with exactly the same proof than in the case $\Omega = I$.

CHAPTER 4

Joint measurability and Bell inequalities.

Quantum entanglement is the source of two of the major consequences of Quantum Mechanics: uncertainty of measurements and non-locality.

Heisenberg posed that some magnitudes – such us momentum and position of particles – cannot be determined simultaneously. The more precise one wants to obtain the outcomes for one of them, the less precise the outcomes for the other will be. This is not the case for non-entangled states, since classical theories could apply in such case.

Joint measurability of observables can be easily proven to be equivalent to commutativity in the case of projective measurements. However, in the case of generalized measurements or positive operator valued measurements this is no longer true. In this chapter, we give several characterizations of joint measurability for this more general type of measurements.

One of the characterizations we get relates joint measurability with non-locality and Bell inequalities. Non-locality of Quantum Mechanics was first noted by Einstein, Podolski and Rosen, understood by them as a lack of completeness of the theory. Later results have led to a deeper understanding of such behaviour. In this direction, Bell proposal of an experiment that would assess the existence of quantum correlations, and CHSH-inequality – from the family of Bell inequalities – have been crucial advances.

Entanglement is necessary for non-locality and the violation of a Bell inequality. However, it is not sufficient, since there exist quantum entangled states that do not violate any Bell inequality. In this chapter we show that the role of joint measurability is quite different: joint measurements never lead to Bell inequality violations, and non-jointly measurable observables can always be used to design CHSH-violating experiments. This direct relationship between joint measurability and non-locality is a novel result never found before between these two very important ingredients of Quantum Theory.

4.1. Bell inequalities, POVMs and semidefinite programming.

Let us start introducing the main objects and tools we deal with in this chapter: Bell inequalities, generalized measurements or POVMs and semidefinite programming.

4.1.1. Bell Inequalities and non-locality. In 1935, Einstein, Podolski and Rosen posed a theoretical experiment that would imply an incompleteness of Quantum Theory: the so-called EPR paradox. Two particles could share some conjugate magnitudes that, as Heisenberg's Uncertaintly Principle predicted, could not be both determined by measuring, and by measuring 'simultaneously' each magnitude in each particle one could somehow break this rule and know both. They concluded that there could exist more local variables in Nature completely out of our control, usually called local hiddel variables (LHV), and such a model could be more complete than quantum theories.

In usual classical theories joint probabilities between distant experiments are completely independent, i.e., $P_{A,B}(a,b) = P_A(a)P_B(b)$. LHV theories allow some additional non-controlled variables $\lambda \in \Omega$, so probabilities in LHV models can be described as convex combinations of product probability distributions

$$P_{A,B}(a,b) = \int_{\Omega} P_A(a,\lambda)P_B(b.\lambda)P_{\Omega}(\lambda)d\lambda \ .$$

However, in 1964 Bell showed that such LHV models could not be compatible with Quantum Mechanics [**15**]. He proved that quantum experiments could lead to some propability outcomes with correlations that would be not possible in any LHV model. The experimental outcomes coming from these models should be bounded by certain values, which some quantum setting could violate. These inequalities are called Bell inequalities.

We describe now the experiment as posed by Clauser et al. [**30**], showing the paradigmatic Bell inequality: the CHSH inequality, which we use in our work. There exist many other Bell inequalities separating classical (LHV) from quantum correlations, depending on the number of measurements and outcomes, the values of the outcomes, the number of parties, etc.

Let Alice and Bob be two distant parties, sharing a maximally entangled bipartite state, say $|\phi\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$. Alice has two measure devices, which implement projective measurements on the orthonormal bases

$$B_+ = \{|0\rangle, |1\rangle\} \text{ and } B_\times = \{|+\rangle, |-\rangle\}.$$

The measurements are represented respectively by the observables

$$A_1 = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = Z \text{ and } A_2 = |+\rangle\langle +| - |-\rangle\langle -| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = X.$$

Therefore, the first vector of each basis is associated to the outcome $+1$, and the second to the outcome -1.

Bob has other two devices, implementing two ±1-valued projective measurements with associated observables

$$B_1 = \frac{-Z - X}{\sqrt{2}} \text{ and } B_2 = \frac{Z - X}{\sqrt{2}}.$$

Since projective measurements can be measured jointly iff they commute, it is clear that A_1 and A_2 cannot be measured jointly, as well as B_1 and B_2. However, Alice and Bob can perform repeated measurements, selecting randomly and independently which measurement to perform, and can try to approximate the expectation value of some quantities. The one we are interested now on is the expectation value of

$$\frac{1}{2}\left(A_1(B_1 + B_2) + A_2(B_1 - B_2)\right).$$

Given classical – determined – values for the outcomes of the measurements, since the only possibilites for B_i are $+1$ or -1, one would have that either $B_1 + B_2 = 0$ or $B_1 - B_2 = 0$. In any case, the expected value of this sum would be upper bounded by 1 (and lower bounded by -1).

However, given a mixed state ρ shared by Alice and Bob, the expectation of this value in Quantum Mechanics is

$$\mathrm{tr}(\rho\mathbb{B}),\ \text{for } \mathbb{B} = \frac{1}{2}(A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2)).$$

$\mathbb{B}$ is called the CHSH operator, relative to A_i and B_i. This expectation value is exactly $\sqrt{2}$ for $\rho = |\phi\rangle\langle\phi|$, with $|\phi\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$, which violates the previous classical bound 1.

Given different observables involving two different parties, say $\{A_i\}_{i=1}^n$ and $\{B_i\}_{i=1}^m$, we can think of calculating the expectation of any linear combination

$$\mathbb{A} = \sum_{i,j} \alpha_{i,j} A_i \otimes B_j,\ \alpha_{i,j} \in \mathbb{R}.$$

Since separable states correspond to those correlations that can be achieved by LHV models, another way to state Bell violations is to decide or quantify the difference between those expected values attainable by separable states from those attainable by general quantum states:

$$\{tr(B\rho), \rho \in \text{sep}\} \subsetneq \{tr(B\rho), \rho \in \text{quant}\}.$$

Any bound of the form $|\mathrm{tr}(A\rho)| \leq C$, for some value C, which is verified for every separable state but not for every quantum state is a bipartite Bell inequality.

It must be noted that entanglement is necessary for the existence of quantum correlations, but there exist entangled states with always lead to classical correlations. This type of entanglement which always give rise to classical probability distributions is called bound entanglement[1].

4.1.2. Generalized measurements. In Chapter 2, devoted to the basic tools in Quantum Mechanics, we already introduced projective measurements. However, a more general setting can be thought of when performing measurements, called generalized measurements. Their need comes from the fact that we may be controlling just a subsystem which is smaller than the real system the projective measurement is taking place onto. Moreover, the measuring devide might be entangled with the system. By tracing out the part of the projective measurement we cannot get information from, we get these generalized measurements.

DEFINITION 4.1.1. Generalized quantum measurements are described by a collection of measurement operators $\{M_{m_i}\}_{i=1}^N$, indexed by the possible real outcomes $\{m_i\}_{i=1}^N$, acting on the state space. If the state of the quantum system prior to the measure is $|\phi\rangle$, then the probability of getting result m_i is given by

$$p(m_i) = \langle\phi|M_{m_i}^\dagger M_{m_i}|\phi\rangle,$$ [2]

[1]In the multipartite setting, bound entanglement is more intricate than in the bipartite setting. Formally, bound entangled states are nonseparable nondistillable states. However, they can violate multipartite Bell inequalities [**36**].

[2]We will use both notations $\dagger$ and $*$ to refer to the Hilbert adjoint operator, following the notation most commonly used in the literature related to each chapter. In this line, $\dagger$ is used along this chapter, and $*$ is used in chapters 5 and 6. In Chapter 6 we will also use a few times $\dagger$ when unitary matrices are acting in the virtual levels. We will recall what $*$ stands for when introducing Matrix Product States in Chapter 5.

and in the case outcome m_i, $i \in \{1,\dots,N\}$, has been obtained, the state of the system after the measurement is

$$\frac{M_{m_i}|\phi\rangle}{\sqrt{\langle\phi|M_{m_i}^\dagger M_{m_i}|\phi\rangle}}$$

The measurement operators must satisfy the completeness equation

$$\sum_{i=1}^{N} M_{m_i}^\dagger M_{m_i} = \mathbb{I}$$

so that the probabilities of the different outcomes sum up to 1.

However, for many applications, the state of the system after the measurement is of little interest. When this happens, all the information we want from the measurement can be obtained from the values of the outcomes m_i and the operators $E_{m_i} = M_{m_i}^\dagger M_{m_i}$, which are positive operators. This leads us to the so-called positive operator valued measurements, or POVMs.

Definition 4.1.2. A POVM is a collection of positive operators $\{E_{m_i}\}_{i=1}^N$, called effect operators and labelled by the possible outcomes of the measurement, such that $\sum_{i=1}^N E_{m_i} = \mathbb{I}$ and $p(m_i) = \langle\phi|E_{m_i}|\phi\rangle$ is the probability of getting the outcome m_i if the system is initially described by $|\phi\rangle$.

How observables are induced by effects is straightforward. From a POVM $\{E_{m_i}\}_{i=1}^N$ we can always build the observable $A = \sum_{i=1}^M m_i E_{m_i}$. If the system is initially in the state $|\phi\rangle$ we have then that the expectation value of the measurement is

$$\langle A\rangle_{|\phi\rangle} = \sum_{i=1}^{N} m_i p(m_i) = \sum_{m=1}^{N} m_i \langle\phi|E_{m_i}|\phi\rangle = \mathrm{tr}(A|\phi\rangle\langle\phi|).$$

For a mixed state ρ we have the analogue expression, $\langle A\rangle_\rho = \mathrm{tr}(A\rho)$.

However, in the opposite direction the relationship is not uniquely defined, since a given observable can be induced by many different effect descompositions. A particular case is that of 'sharp' observables, described by Hermitian operators whose spectra represent the possible measurement outcomes, and the projections associated to different eigenspaces are the effect operators. In this last case the decomposition is essentially unique.

4.1.3. Semidefinite programming. The last notion we need is that of semidefinite programming. A semidefinite programming problem is a convex optimization problem in which the objective function is linear and the feasible region is determined by linear matrix constraints:

$$\begin{aligned} &\text{calculate} && \inf_{x\in\mathbb{R}^n} \langle c|x\rangle \\ &\text{subject to} && \sum_i x_i F_i \geq C, \end{aligned}$$

where the matrices F_i and C must be Hermitian.

There is a dual problem to this one

$$\begin{aligned} &\text{calculate} && \sup_{X\geq 0} \mathrm{tr}(CX) \\ &\text{subject to} && \mathrm{tr}(XF_i) = c_i. \end{aligned}$$

The restrictions of the type $A \geq B$ between Hermitian matrices means that $A - B$ is semidefinite positive.

As in the case of linear problems, the dual problem of a semidefinite programming problem is again a SDP problem. And in the case one of the problems is strictly feasible, then the other also attains its extremum and both have the same result.

This class of problems includes, among many others, every linear programming problem. The feasible region is a convex set, but since the boundary is not determined by linear constraints simplex methods are not valid for finding a solution. However, most interior point methods are still valid for approximating efficiently the optimum. In fact, semidefinite programming has polynomial worst-case complexity [**47**].

4.2. Characterizations of the joint measurability problem.

4.2.1. Sharp observables. The case of sharp observables is the same as the case of projective or von Neumann measurements. The Hermitian operators defining sharp observables can be diagonalized, and the effect operators correspond to the projectors onto the different eigenspaces associated to the Hermitian operators.

The relationship between joint measurability and violation of Bell inequalities is well-known in the case of projective measurements. Two projective measurements can be performed jointly iff their associated observables are simultaneously diagonalizable.

In the case we have a set of sharp observables E_i which are not commuting, there should exist at least one non-commuting pair: let us say E_1 and E_2. Similarly, such a pair of operators contains at least one non-commuting pair of spectral projections. By relabelling outcomes we can therefore always build a pair of non-commuting ± 1-valued sharp observables A_1, A_2 from a set of incompatible von Neumann measurements.

It is easy to derive the relationship between joint measurability and violation of Bell inequalities, since for each such pair of non-jointly measurable observables we can find a bipartite quantum state ρ and ± 1-valued sharp observables B_1, B_2 which violate the CHSH inequality $|\langle \mathbb{B} \rangle_\rho| \leq 1$ where

$$\mathbb{B} = \frac{1}{2}\Big[A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2)\Big].$$

To this end note that for some given observables the CHSH inequality holds for all quantum states iff all its eigenvalues lie between -1 and 1, that is, $-\mathbb{I} \leq \mathbb{B} \leq \mathbb{I}$, or equivalently, $\mathbb{B}^2 \leq \mathbb{I}$.

Using that the observables have unit square one gets [**71**]

$$\mathbb{B}^2 = \mathbb{I} - \frac{1}{4}[A_1, A_2] \otimes [B_1, B_2].$$

Since the tensor product of the commutators is Hermitian and traceless, $\mathbb{B}^2$ has an eigenvalue larger than one iff the commutators do not vanish. Hence any non-commuting pair B_1, B_2 enable a violation of the CHSH inequality.

Some easy bounds can be obtained from this fact. For Alice and Bob measuring the same observables, $B_i = A_i$, the optimal state – the eigenstate associated to the eigenvalue with maximum absolute value – gives the quantitative relation

$$\max_\rho |\langle \mathbb{B} \rangle_\rho| = \sqrt{1 + \|[A_1, A_2]\|^2/4}.$$

If we are interested in the maximal violation than can be obtained given A_1 and A_2 we need an optimal choice of the $B's$ ($\|[B_1, B_2]\| = 2$, e.g. by setting $B_1 = X$ and $B_2 = Z$) to get

$$\max_{\rho, B_1, B_2} \left|\langle \mathbb{B} \rangle_\rho\right| = \sqrt{1 + \frac{1}{2}\|[A_1, A_2]\|}\,.$$

4.2.2. General measurements. Our aim is to study the joint measurability problem in the most general case: that of POVMs. Two dichotomic POVMS/effects are jointly measurable if there exists another measurement from which we can extract all the information we could get from both. The new measurement must let us recover the original probability outcomes for both effects and for every possible state. Let us now state formally what we understand as joint measurability in this case.

Definition 4.2.1. Let A_1 and A_2 be described by d-dimensional POVMs, i.e., pairs of positive semidefinite 'effect' operators $\{Q, \mathbb{I} - Q\}$ and $\{P, \mathbb{I} - P\}$ whose expectation values give the probabilities of the assigned measurement outcomes. These observables are jointly measurable within Quantum Mechanics iff there is a measurement with four outcomes corresponding to four positive operators R_{ij}, $(i, j = \pm)$ with correct 'marginals' $R_{++} + R_{+-} = Q$ and $R_{++} + R_{-+} = P$.

Beyond the case of qubits [**23**] there is no previous explicit characterization of jointly measurable observables known, but we can easily get an implicit one:

Proposition 4.2.2. *Two observables characterized by the effects P and Q are jointly measurable iff there is a positive semidefinite operator S satisfying $Q + P - \mathbb{I} \leq S \leq P, Q$.*

Proof. Necessity of this condition is proven by taking $S = R_{++}$ and sufficiency by simply constructing the other R's from the given relations: $R_{+-} = Q - S$, $R_{-+} = P - S$, and $R_{--} = \mathbb{I} - Q - P + S$, all of which result semidefinite positive and bounded by $\mathbb{I}$. □

The existence of such S given P and Q is not always easy since the set of operators with the partial order $\leq$ does not form a lattice. Were this the case, it would be enough to find $\min\{P, Q\}$ and check whether this operator satisfy being positive and greater that $Q + P - \mathbb{I}$. This can be done easily in the case of projective measurements, leading to the characterization described before.

Despite this difficulty, we can rephrase Prop. 4.2.2 as a semidefinite program [**123**], and therefore it can be decided efficiently numerically.

Proposition 4.2.3. *Two observables described by effect operators P and Q are jointly measurable iff the solution of the semidefinite program*

$$\lambda_0 = \inf\{\, \lambda \in \mathbb{R}\, |Q + P \leq \lambda \mathbb{I} + S\}$$

subject to the constraints $0 \leq S \leq Q, P$ is lower or equal to 1.

PROOF. The equivalence between this proposition and Prop. 4.2.2 is inmediate, since for a solution $\lambda_0 \leq 1$ we would have $Q + P - \mathbb{I} \leq Q + P - \lambda_0 \mathbb{I} \leq S$. The only additonal fact in this statement is the fact that the problem can be casted as a semidefinite program.

Let us consider an Hermitian basis G_i of the dimension of P and Q, and let us express the unknown matrix S as $S = \sum_i x_i G_i$. Then, by setting

$$\begin{aligned} C &= (Q+P) \oplus 0 \oplus (-Q) \oplus (-P), \\ F_0 &= \mathbb{I} \oplus 0 \oplus 0 \oplus 0, \\ F_i &= G_i \oplus G_i \oplus (-G_i) \oplus (-G_i), \; i \geq 1, \\ c_0 &= 1, \\ c_i &= 0, \quad i \geq 1, \text{ and} \\ x_0 &= \lambda \end{aligned}$$

we get an expression of the problem in the proposition as a semidefinite program. □

If we consider the dual problem we get the following characterization of joint measurability

PROPOSITION 4.2.4. *Two observables described by effect operators P and Q are jointly measurable iff the supremum*

$$\lambda_0^* = \sup_{X,Y,Z \geq 0} \operatorname{tr}\left(X(Q+P-\mathbb{I})\right) - tr(QY) - tr(PZ),$$

subject to $X \leq (Y+Z)$ and $\operatorname{tr}(Y+Z) = 1$, is not positive.

PROOF. Taking the semidefinite program in the proof of previous proposition, we would have that the dual problem is

$$\lambda_0 = \sup_{X \oplus T \oplus Y \oplus Z \geq 0} \operatorname{tr}\left(X(Q+P)\right) - \operatorname{tr}(YQ) - \operatorname{tr}(PZ), \tag{11}$$

subject to $\operatorname{tr}(X) = 1$, and $\operatorname{tr}((X+T-Y-Z)G_i) = 0$, $i > 0$.

Note that, since T plays no role in the objective function, for every possible feasible values X, Y, Z we can set $T = Y + Z - X$, and in this way $\operatorname{tr}((X+T-Y-Z)G_i) = 0$, $i > 0$, is automatically satisfied. Note also that the conditions $T \geq 0$ and $Y + Z \geq X$ are equivalent in this case. Checking whether this last problem is lower or greater than 1 is equivalent to checking whether

$$\lambda_0 - 1 = \sup_{X,Y,Z \geq 0} \operatorname{tr}\left(X(Q+P-\mathbb{I})\right) - \operatorname{tr}(YQ) - \operatorname{tr}(PZ),$$

subject to $\operatorname{tr}(X) = 1$, and $Y + Z \geq X$, is negative or positive.

At this point we have an homogeneous problem, therefore we can choose to normalize $Y + Z$ instead of X, leading to the problem in the statement of the proposition:

$$\lambda_0^* = \sup_{X,Y,Z \geq 0} \operatorname{tr}\left(X(Q+P-\mathbb{I})\right) - tr(QY) - tr(PZ),$$

subject to $X \leq (Y+Z)$ and $\operatorname{tr}(Y+Z) = 1$. □

Our aim now is to show how λ_0^* is related to the maximal violation of the CHSH inequality to which Q and P can lead and, using this insight, to provide a simple way of computing it, without the need of setting up a semidefinite programming algorithm. Our main result is the following duality between the questions of whether two observables are jointly measurable and whether they enable a violation of the CHSH inequality:

THEOREM 4.2.5 (CHSH). *Two measurements characterized by effect operators Q and P are not jointly measurable iff they enable the violation of a CHSH inequality. Quantitatively,*

$$\sup_{\rho,B_1,B_2} \left|\langle \mathbb{B}_\rho\rangle\right| = 1 + 2\lambda_0^*, \tag{12}$$

whereas

$$\sup_{\rho\in\text{sep},B_1,B_2} \left|\langle \mathbb{B}_\rho\rangle\right| \leq 1. \tag{13}$$

PROOF. We begin by rewriting the constraints in the dual problem from Proposition 4.2.4 by introducing $\rho := Z + Y$, $\tilde{Q} := \rho^{-1/2}X\rho^{-1/2}$ and $\tilde{P} := \rho^{-1/2}Y\rho^{-1/2}$, using the pseudo-inverse when necessary. The constraints in this problem translate then to $0 \leq \tilde{Q}, \tilde{P} \leq \mathbb{I}$ – i.e., $\tilde{Q}$ and $\tilde{P}$ being effect operators – and ρ being a density operator – $\operatorname{tr}(\rho) = 1$. We then exploit that the latter is the reduced density operator of a normalized pure state $|\psi\rangle := (\sqrt{\rho}\otimes\mathbb{I})\sum_{i=1}^{d}|ii\rangle$ and that for instance $\operatorname{tr}(QY) = \langle\psi|Q\otimes\tilde{P}^T|\psi\rangle$. In this way we obtain

$$\lambda_0^* = \sup\, \langle\psi\big|(Q+P-\mathbb{I})\otimes\tilde{Q} - Q\otimes\tilde{P} - P\otimes(\mathbb{I}-\tilde{P})\big|\psi\rangle,$$

where the supremum is taken over all admissible effect operators $\tilde{Q},\tilde{P}$ and state vectors $|\psi\rangle$.

If we now set the observables $A_1 = \mathbb{I} - 2P$, $A_2 = 2Q - \mathbb{I}$, $B_1 = \mathbb{I} - 2\tilde{P}$ and $B_2 = \mathbb{I} - 2\tilde{Q}$, and $\mathbb{B} = (A_1\otimes(B_1+B_2) + A_2\otimes(B_1-B_2))/2$, we get the expression

$$\lambda_0^* = \sup\, \langle\psi|\mathbb{B}-\mathbb{I}|\psi\rangle/2, \tag{14}$$

with the same conditions as before on $\tilde{Q},\tilde{P}$ and $|\psi\rangle$.

The problem (14) can be also rephrased as

$$\lambda_0^* = \sup\, \langle\psi\big|(Q+P-\mathbb{I})\otimes(\mathbb{I}-\tilde{Q}) - Q\otimes(\mathbb{I}-\tilde{P}) - P\otimes\tilde{P}\big|\psi\rangle,$$

where the supremum is taken again over all admissible effect operators $\tilde{Q},\tilde{P}$ and state vectors $|\psi\rangle$.

This last version of the problem leads to the expression

$$\lambda_0^* = \sup\, \langle\psi|-\mathbb{B}-\mathbb{I}|\psi\rangle/2. \tag{15}$$

From equations (14) and (15) we can finally get the statement in the theorem. Note that, due to convexity, the supremum over all mixed states coincides with the supremum over all pure states, which are the extremal points of the set of mixed states.

□

THEOREM 4.2.6. *The supremum can be computed as $\lambda_0^* = \max_{\phi\in[0,\pi]}\mu(\phi)$ where $\mu(\phi)$ is the largest eigenvalue of*

$$(Q+P-\mathbb{I})\otimes\begin{pmatrix} c^2 & cs \\ cs & s^2\end{pmatrix} - Q\oplus P, \tag{16}$$

with $c = \cos(\phi)$ and $s = \sin(\phi)$.

PROOF. If we consider the problem (14) we can use that, due to convexity, this extremal value is attained for $\tilde{P}$ and $\tilde{Q}$ being projections.

Since two projections can be unitarily diagonalized simultaneously [**54**] up to blocks of size at most 2×2, we obtain (again employing convexity) the same maximal violation when restricting to $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^2$.

And, as the maximum over $|\psi\rangle$ is nothing but computing the largest eigenvalue we can make further use of the unitary freedom we have to fix one of the observables, say $\tilde{P} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and make $\tilde{Q}$ a real projector with non-negative entries, which finally leads to the expression in (16). □

Two general observables. In a similar vein we can now treat more general scenarios. All of them have a strictly feasible dual so that equality holds between primal and dual problem.

We can consider two $N-$outcome arbitrary observables which are characterized by two sets of effect operators $\{Q_i\}$,$\{P_j\}$ with $i, j = 1, \dots, N$. These are jointly measurable iff we can find $\{R_{ij} \geq 0\}$ such that $\sum_i R_{ij} = P_j$ and $\sum_j R_{ij} = Q_i$.

One way, analogous to the previous one, to express this as a semidefinite program is to minimize $\lambda \in \mathbb{R}$ w.r.t. to $\{R_{ij} \geq 0\}$ such that

$$\sum_{i=1}^{N-1} Q_i + \sum_{j=1}^{N-1} P_j \leq \lambda \mathbb{I} + \sum_{i,j=1}^{N-1} R_{ij}$$

and $P_j \geq \sum_{i=1}^{N-1} R_{ij}$ and $Q_i \geq \sum_{j=1}^{N-1} R_{ij}$ for all i, j.

The corresponding dual is

$$\lambda_0 = \sup_{\rho, Y_i, Z_j \geq 0} \sum_{i=1}^{N-1} \mathrm{tr}(Q_i(\rho - Y_i) + P_i(\rho - Z_i)),$$

subject to the additional constraints $\rho \leq Y_i + Z_j$ for all i, j and ρ being a density operator. Note the similarity between this problem and the one from eq. (11).

Several dichotomic observables. We can also consider several dichotomic observables. Let M two-valued observables be characterized by effect operators $0 \leq T_\alpha \leq \mathbb{I}$, $\alpha = 1, \dots, M$. We will denote the effect operators of the sought joint observable by R_i using a multi-index $i \in \{0,1\}^M$ with $|i| := \sum_\alpha i_\alpha$. T_α will be identified with the sum of all R_i for which $i_\alpha = 1$.

The existence of a joint observable can then be expressed in terms of the constraints $R_i \geq 0$, $\forall i$, and

$$\sum_{|i|>1} R_i \delta_{i_\alpha,1} \leq T_\alpha,$$

$$\sum_\alpha T_\alpha \leq \mathbb{I} + \sum_{|i|\geq 1} (|i| - 1) R_i,$$

for every α.

This problem can be rephrased again as a quantitative semidefinite program by replacing $\mathbb{I} \to \lambda\mathbb{I}$ and minimizing λ. Again the minimum λ_0 can as well be obtained from the dual:

$$\lambda_0 = \sup_{\rho,\{X_\alpha \geq 0\}} \sum_\alpha \mathrm{tr}\left(T_\alpha(\rho - X_\alpha)\right), \quad \text{subject to} \quad \forall i: \ (|i| - 1)\rho \leq \sum_\alpha \delta_{i_\alpha,1} X_\alpha, \tag{17}$$

where ρ is constrained to be a density operator.

4.3. Bell inequalities and no-signalling.

One of the consequences of the previous results is that measurements which cannot be measured jointly in Quantum Mechanics cannot be measured jointly within any no-signalling theory. No-signalling theories are those for which the probabilities of measurements in distant places which are performed 'simultaneously' – none of them lies in the casual cone of the other – are independent of the other's choice of the measurement device. That is, for a joint probability distribution[3] $\{P(a,b|x,y)\}_{x,y;a,b=1}^{N;k}$, the marginals must verify

$$\sum_{a=1}^{k} P(a,b|x,y) = P(b|y), \ \forall x \ ,$$

$$\sum_{b=1}^{k} P(a,b|x,y) = P(a|x), \ \forall y \ .$$

This consequence is due to the relationship found between joint measurability and Bell inequalities, and the already known link between Bell inequalities and no-signalling, which we explain in this chapter. Variants of these arguments, or its main ingredients, can be found in [**43, 79, 133, 136**].

Suppose Alice can jointly measure two observables, which are labelled by A_1 and A_2, and yield outcomes a_1, a_2 with probability $P(a_1, a_2)$. If Bob, at a distance, measures an observable B_1 with outcome b_1, then they observe in a statistical experiment a joint probability distribution $P(a_1, a_2, b_1|B_1)$ so that

$$P(a_1, a_2) = \sum_{b_1} P(a_1, a_2, b_1|B_1).$$

However, in a no-signalling theory this has to be independent of Bob's chosen observable, i.e., a possibly measured $P(a_1, a_2, b_2|B_2)$ has to have the same marginal $P(a_1, a_2)$. Assume that Bob chooses B_1 or B_2 at random so that they measure both triple distributions. From these we can write down a joint distribution

$$P(a_1, a_2, b_1, b_2) := \frac{P(a_1, a_2, b_1|B_1)P(a_1, a_2, b_2|B_2)}{P(a_1, a_2)}, \tag{18}$$

which by construction correctly returns all measured distributions as marginals. As a result, the possibility of jointly measuring A_1 and A_2 implies a joint probability distribution (18) if the no-signalling condition is invoked. A joint distribution, in turn, implies that

[3] As common in classical probability theory we use the notation $p(\cdot|\cdot)$ where right of the dash is the *condition* which the probability is subject to. In our case this is the observable which is measured.

no Bell inequality can be violated. So if a Bell inequality is violated, then either A_1 and A_2 are not jointly measurable, or the no-signalling condition is violated.

Note that this argument works independent of the numbers of measurement outcomes or observables.

CHAPTER 5

Uncle Hamiltonians for Matrix Product States.

In this chapter we move from bipartite systems to multipartite systems, studying problems in many-body physics, of particular importance in quantum statistics and condensed matter. The problems we tackle are not related to multipartite entanglement, but to bipartite entanglement between two disjoint regions, which is also a very interesting problem in this setting.

Most physically relevant states show a property called area law for the entropy of entanglement: if we divide the complete system into two regions the entropy is related to the size of the boundary separating the two regions instead of to the size of the regions, as it happens with generic random states. The area law is due to the local behaviour of natural interactions, and is related to the presence of fast decaying correlations between particles and to gapped Hamiltonians.

The tools we use in this chapter are Matrix Product States (MPSs) and some related Hamiltonians. MPSs satisfy this area law by construction, and in one-dimensional lattices they have been identified as a class of states which approximates ground states of locally interacting systems. Powerful numerical methods based on renormalization groups (DMRG [**134**]) have been designed, and their success is supported on theoretical results such as [**56**]. Matrix Product states are described by some sets of matrices, giving as a consequence that only polinomially many parameters – instead of the exponentially many coefficients that would needed to describe a generic state – need to be handled in order to apply such methods.

MPSs come together with some local Hamiltonians, the parent Hamiltonians, for which the MPSs are exact ground states, thus providing quasi-exactly solvable models in many-body systems. Conditions are known for them to be the unique ground state of their parent Hamiltonians – injectivity – and, for translationally invariant states, parent Hamiltonians are known to be gapped over the ground state level.

The aim of this chapter is to deepen the study of the relationship between MPSs and their parent Hamiltonians. It was noted in [**26**], in a 2-dimensional setting, that the parent Hamiltonian construction is not continuous, showing how different changes in the tensor description affect the topological entanglement entropy of the system when the symmetry of the tensor description is broken.

Therefore, we consider small linear perturbations of the matrix description of every MPS and study when the parent Hamiltonian construction is continuous – i.e. physical – under such perturbation, identyfying injective MPSs as those for which the construction is robust.

In the case of lack of robustness – non-injective MPSs–, we consider the limit as the perturbation vanishes to construct the corresponding uncle Hamiltonians and study their properties for almost every perturbation. This way we are able to find new Hamiltonians for the same states with many common properties to the parent Hamiltonians, but with completely different spectral properties: both parent and uncle Hamiltonians are local – with the same interaction length – and frustration free, and have the same ground state space for closed chains; on the other hand, the uncle Hamiltonian is gapless whereas the parent Hamiltonian is gapped.

We also consider the problem on infinite open chains, what is called the thermodynamic limit – with applications to the study of phases of matter and criticality –, showing also that they have the same ground state space – even though this property is not true for finite open chains – and the spectrum of the uncle Hamiltonian is the positive real line, which contrasts with the gap the parent Hamiltonian exhibits. This study let us get some more information about the spectra of the uncle Hamiltonians for finite open and closed chains: they are not only gapless, but also their spectra tend to be dense in $\mathbb{R}^+$ as the size of the chain grows.

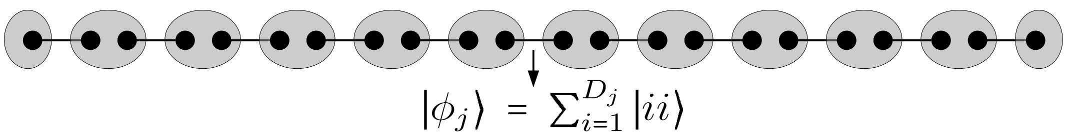
Finally, we also provide uncle Hamiltonians for injective MPSs and study their properties. They are also gapless and their spectra in the thermodynamic limit is $\mathbb{R}^+$, but they differ from those for non-injective MPSs in the fact that their ground state space is not the same as the one of the parent Hamiltonian for closed chains, even though it is also the same in the thermodynamic limit.

5.1. Matrix Product States and parent Hamiltonians.

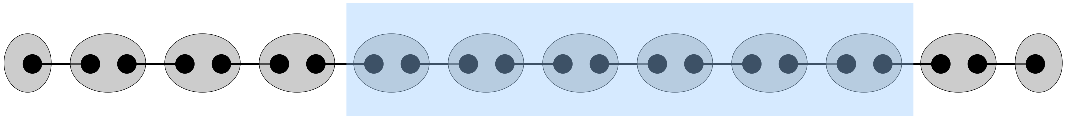
In this section we provide the basic definitions and tools related to Matrix Product States.

5.1.1. Basic definitions. Matrix Product States can be constructed starting from this idea of area law: The entropy between two regions depends on the size of boundary and not on the bulk.

Let us consider a set of sites disposed in a one-dimensional lattice, i.e. in a line, and let us first consider that between every couple of neighbouring sites there is a maximally entangled pair of arbitrary dimension, $|\phi_j\rangle = \sum_{i=1}^{D_j} |ii\rangle$. We will often deal with unnormalized states. Therefore, we will need to normalize whenever this issue is relevant (e.g., when calculating expectations values, energies, etc.).



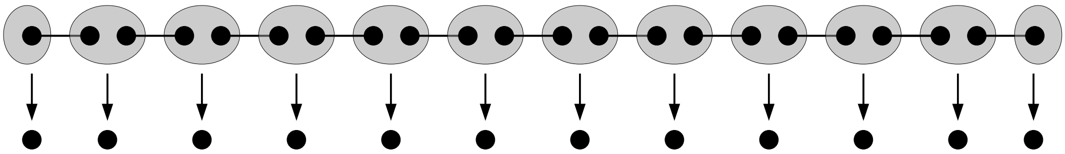
The complete system is then described by the state $|\Phi\rangle = \otimes_j |\phi_j\rangle$, which already satisfies the area law. For every cut into two regions, the entanglement entropy between these two regions only depends on the number of cuts we have made. If we set for example the following cut between the coloured region and the other one



the entropy depends on the two cuts j_1 and j_2 we have made: $S = \log D_{j_1} + \log D_{j_2}$.

In order to get the entire family of Matrix Product States, we need to apply arbitrary linear maps $P_k : \mathbb{C}^{D_{j_{k-1}}} \otimes \mathbb{C}^{D_{j_k}} \to \mathbb{C}^{d_k}$ at every site. The final state can be written as

$$|\varphi\rangle = \otimes_k P_k |\Phi\rangle.$$



The map at every site k can be interpreted as a set $\{A_i^{[k]}\}_i$ of $D_{j_{k-1}} \times D_{j_k}$ matrices such that

$$P_k = \sum_{i,\alpha,\beta} A^{[k]}_{i,\alpha,\beta} |i\rangle\langle\alpha, \beta|. \tag{19}$$

From this matrices the vector $|\varphi\rangle$ can also be described as stated in the following definition.

Definition 5.1.1. A pure state $|\varphi\rangle \in \otimes_{j=1}^{L} \mathbb{C}^{d_j}$ is called a Matrix Product State (MPS) with open boundary conditions if it can be written as

$$|\varphi\rangle = \sum_{i_1,\dots,i_L} A^{[1]}_{i_1} A^{[2]}_{i_2} \cdots A^{[L-1]}_{i_{L-1}} A^{[L]}_{i_L} |i_1 \cdots i_L\rangle$$

where the $A^{[j]}_{i_j}$ are $D_{j-1} \times D_j$ matrices, with $D_0 = D_L = 1$, for $i_j = 1, \dots, d_j$. The value $D = \max_j D_j$ will be called the bond dimension of this MPS representation. The different $\mathbb{C}^{d_j}$ will be referred to as physical sites, and the values d_j will be the respective physical dimensions.

This is the most general type of MPS. Note that any MPS may admit many different representations. An easy example comes from just taking an invertible matrix C and setting $B^{[j]}_i = A^{[j]}_i C$ and $B^{[j+1]}_k = C^{-1} A^{[j+1]}_k$, for every possible i and k.

Every finite dimensional state can be modelled as an MPS if we take high enough values for the bond dimension D. However, their importance lies on the fact that ground states of one-dimensional local gapped Hamiltonians can be approximated efficiently by Matrix Product States keeping the bond dimension relatively low, and therefore using only polynomial many coefficients instead of the exponentially many one would need to describe them [**19, 56, 72**]. This is what makes MPSs a powerful numerical tool. In addition, many interesting states have an exact MPS description with very low bond dimension, such as product states, GHZ states, AKLT states, W states, etc.

Example 5.1.2. Any product state $|\varphi\rangle = \otimes_j \sum_i a^{[j]}_i |i\rangle$ can be described as MPSs by taking $A^{[j]}_i = a^{[j]}_i$.

EXAMPLE 5.1.3. The unnormalized n-qubit W state is

$$|\mathrm{W}\rangle = |1000\cdots0\rangle + |0100\cdots0\rangle + |0010\cdots0\rangle + \cdots + |0000\cdots1\rangle,$$

and it can be expressed as an MPS by taking

$$A_0^{[0]} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ A_1^{[0]} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

$$A_0^{[i]} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ A_1^{[i]} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},\ i = 2, \ldots, L-1,$$

$$A_0^{[L]} = \begin{pmatrix} 0 & 1 \end{pmatrix},\ A_1^{[L]} = \begin{pmatrix} 1 & 0 \end{pmatrix}.$$

In the case every physical site has the same dimension – $d_k = d\ \forall k$ – there exists a very interesting class of states, representing homogeneus matter, which are the translationally invariant states.

DEFINITION 5.1.4. A state $|\varphi\rangle \in \otimes_{j=1}^{L}\mathbb{C}^d$ is called translationally invariant (t.i.) if it is invariant under the translation map defined by

$$\tau(|i_1\cdots i_{L-1}i_L\rangle) = |i_L i_1\cdots i_{L-1}\rangle$$

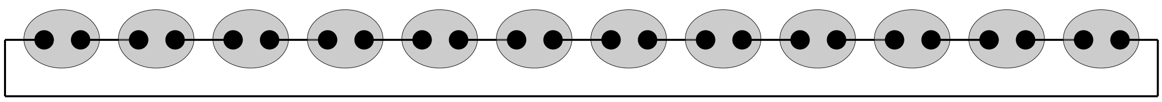
For these states one can always find a matrix representation with the same set of matrices at every site.

DEFINITION 5.1.5. A state $|\varphi\rangle \in \otimes_{j=1}^{L}\mathbb{C}^d$ is called a translationally invariant MPS (with t.i. representation) if it can be written as

$$|M(A)\rangle = \sum_{i_1,\ldots,i_L} \mathrm{tr}(A_{i_1}A_{i_2}\cdots A_{i_L})|i_1\cdots i_L\rangle,$$

for a given set of square matrices $\{A_i\}_{i=1}^{d}$. Such MPSs are said to have periodic or closed boundary conditions.

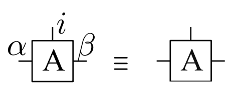
From now on we will be always be referring to this type of MPSs, and every time we say MPS we would be omitting that it is translationally invariant. The picture this corresponds to is that of the systems arranged in a one-dimensional circular lattice, with the first system interacting with the last system.



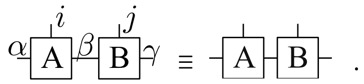
EXAMPLE 5.1.6. The GHZ state $|00\cdots0\rangle + |11\cdots1\rangle$ can be described as a t.i. MPS by taking $A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $A_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

The W state described before has also t.i. MPS descriptions, but they depend on the size of the chain [**112**]

5.1.2. Graphical representation. In order to represent the tensors A as three-index tensors we will use a graphical notation: a k-index tensor will be represented as a box with k legs. The tensor A defining an MPS would then be

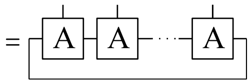
$\{A_i\}_i =$  , where the labels of the indices are usually omitted. The vertical legs will correspond to physical indices, labelling the different matrices, and horizontal legs to virtual ones, labelling rows and columns in the matrices.

The contraction of different tensors, i.e., summing over a common index, is denoted in this graphical language by concatenating the corresponding indices. $\sum_\beta (A_i)_{\alpha\beta}(B_j)_{\beta\gamma}$ is written as



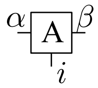
In mathematical language this contraction will be denoted as $A \overset{c}{-} B$.

In this graphical notation an MPS defined by a tensor A is written as

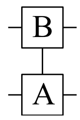
$$|M(A)\rangle =$$  .

The contracion of horizontal legs in this setting corresponds to matrix multiplications. And the contraction of the first horizontal leg with the last one is performed by taking the trace.

In order to compute norms, expectation values, etc., we need to contract tensors with their adjoints. Tensors with legs pointing down are always complex conjugated[1],

 $$\equiv (\bar{A}_i)_{\alpha\beta} \equiv (A_i^*)_{\beta\alpha} \; .$$

An object of particular interest is the 'transfer operator'

$$E_A^B =$$  ,

which we will sometimes interpret as a map from the right to the left indices,

$$E_A^B : X \mapsto \sum_i A_i X B_i^* .$$

5.1.3. Normal form and injectivity. We already stated that the same state can have many different MPS representations. However, some of them are specially well behaved for our purposes. Let us introduce them.

One of the key ingredients is that MPSs are stable under blocking: If we e.g. block pairs of physical sites, $j_k \equiv (i_{2k-1}, i_{2k})$, the state can again be expressed as an MPS in the blocked indices, with tensors $A_{j_k} \equiv A_{i_{2k-1}} \overset{c}{-} A_{i_{2k}}$.

By blocking a finite number of sites [**112**] and appropriate gauge transformations (i.e. multiplying by invertible matrices), any MPS can be brought into a standard form [**41, 101**].

THEOREM 5.1.7 (Standard form for MPS [**41, 101**], injectivity). *After blocking, any MPS can be written in a standard form where the matrices A_i have the following properties:*

(1) *The A_i are block-diagonal: $A_i = \oplus_{j=1}^{\mathcal{D}} A_i^j \otimes \Gamma_j$, where $A_i^j \in \mathcal{M}_{l_j}$ (the space of $l_j \times l_j$ matrices) and the Γ_j are positive diagonal matrices.*

[1]Throughout, $\bar{\cdot}$ will denote the complex conjugate and $\cdot^*$ the adjoint operator.

(2) *The A_i span the space of block-diagonal matrices:* $\mathrm{span}_i A_i = \bigoplus_{j=1}^{\mathcal{D}} \mathcal{M}_{l_j} \otimes \Gamma_j$.

(3) *For all j, the map $\mathcal{E}_j := E_{A^j}^{A^j}$ has spectral radius one, with 1 as the unique eigenvalue of modulus 1, and with eigenvectors $\mathcal{E}_j(\mathbb{I}) = \mathbb{I}$ and $\mathcal{E}_j^*(\Lambda_A^j) = \Lambda_A^j$, where $\Lambda_A^j > 0$, $\mathrm{tr}(\Lambda_A^j) = 1$.*

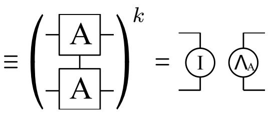
Property 2 with every $\Gamma_j = 1$ is called block-injectivity; in particular, if $\mathcal{D} = 1$, and $\Gamma_1 = 1$, A is called injective.

For the rest of the chapter, we will always consider MPS in this standard form[2].

Note that the role of the matrices Γ_j in this standard form is just counting possible repeated blocks, which essentially does not change the MPS beyond some scaling. Consequently, after blocking every MPS can be considered either as injective or as block-injective.

The uniqueness of the fixed points in each block leads to the following results concerning the transfer operators, which we shall use later.

LEMMA 5.1.8. *Let A denote an injective block of an MPS. Then*

(20) $$(E_A^A)^k \equiv$$  $$+\, O(e^{-k}) \ .$$

Note that $O(e^{-k})$ denotes a bound up to a constant in the exponent. This notation will be used throughout this work.

LEMMA 5.1.9. *Under the conditions of Theorem 5.1.7, the spectral radius $\rho(E_{A^j}^{A^i}) < 1$ for $i \neq j$.*

PROOF. Let us suppose there exists a matrix X such that $E_{A^j}^{A^i} = \sum_k A_k^j X (A_k^i)^* = \lambda X$. By using Cauchy-Schwarz inequality, we would have that

$$|\lambda|\,\mathrm{tr}(X\Lambda_{A^i}X^*) = |\sum_k \mathrm{tr}(A_k^j X (A_k^i)^* \Lambda_{A^i} X^*)| <$$

$$< \left(\sum_k \mathrm{tr}(X(A_k^i)^*\Lambda_{A^i}A_k^i X^*)\right)^{1/2} \left(\sum_k \mathrm{tr}((A_k^j)^* X \Lambda_{A^i} X^* A_k^j)\right)^{1/2} = \mathrm{tr}(X\Lambda_{A^i}X^*),$$

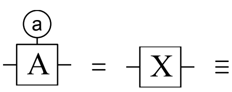
and therefore for any eigenvalue we would have $|\lambda| < 1$. Note that the inequality is strict since we have that $\mathrm{span}\{\langle k|A^i|l\rangle\} \cap \mathrm{span}\{\langle m|A^j|n\rangle\} = \{0\}$ due to block-injectivity. $\square$

We will also need the following consequences of injectivity of tensors.

LEMMA 5.1.10 (Consequences of injectivity). *The following three properties are equivalent, $1 \Leftrightarrow 2 \Leftrightarrow 3$:*

(1) *A is injective.*

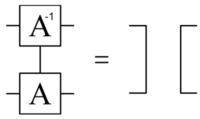
(2) *For any X, there exists an $|a\rangle$ such that*

(21) $$\sum_i \langle a|i\rangle A_i \equiv$$  $$\equiv X \ .$$

[2]Some other tensors will appear, which will not be in this standard form. In particular, note that the 'uncle' tensor and the perturbation tensor will not be MPS tensors.

(3) *There exists a tensor A^{-1}, 'left inverse to A', such that*

(22) $$\sum_i (A_i)_{\alpha\beta}((A^{-1})_i)_{\alpha'\beta'} \equiv$$

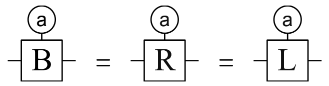


$$= \delta_{\alpha\alpha'}\delta_{\beta\beta'} \ .$$

Also, the following three are equivalent, $4 \Leftrightarrow 5 \Leftrightarrow 6$:

(4) *The block matrix $\left(\begin{smallmatrix} A & R \\ L & B \end{smallmatrix}\right)$ is injective*

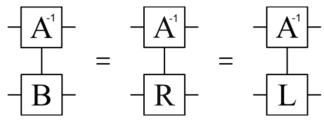
(5) *For any X of the dimensions of A, there exists an $|a\rangle$ such that (21) holds, and additionally*



$$= 0 \ ,$$

and the corresponding statement holds for the other three blocks.

(6) *There exists a tensor A^{-1} such that (22) holds, and additionally*



$$= 0 \ ,$$

and the corresponding statement holds for the other three blocks.

Proof. $1 \Leftrightarrow 2$ since by definition, injectivity means that the A_i span the whole matrix algebra.

$2 \Rightarrow 3$ by taking $|a_{\alpha\beta}\rangle$ such that in (21), $X = |\alpha\rangle\langle\beta|$, and choosing $((A^{-1})_i)_{\alpha\beta} = \langle a_{\alpha\beta}|i\rangle$.

$3 \Rightarrow 2$ by setting $\langle a|i\rangle = \mathrm{tr}((A^{-1})_i X^T)$.

$4 \Rightarrow 5$ by considering equivalence between 1 and 2 and the matrix

$$\tilde{X} = \begin{pmatrix} X & 0 \\ 0 & 0 \end{pmatrix},$$

or the corresponding matrices for the other blocks.

$5 \Rightarrow 4$ since any matrix can be block-decomposed as

$$\begin{pmatrix} X & Z \\ W & Y \end{pmatrix},$$

and for these blocks there exist vectors $|a_X\rangle, |b_Y\rangle, |r_Z\rangle, |l_W\rangle$ that give rise to X, Y, Z and W when applied to A, B, R and L respectively (i.e., operated as in 2 and 5), and 0 when applied to the other blocks. Thus we can consider the sum $|a_X\rangle + |b_Y\rangle + |r_Z\rangle + |l_W\rangle$ to satisfy condition 2, and therefore injectivity of tensor in 4.

$5 \Rightarrow 6$ by defining $|a_{\alpha\beta}\rangle$ such that in (21) $X = |\alpha\rangle\langle\beta|$ if both indices correspond to the A block or 0 otherwise, and choosing $((A^{-1})_i)_{\alpha\beta} = \langle a_{\alpha\beta}|i\rangle$.

And finally $6 \Rightarrow 5$ by setting $\langle a|i\rangle = \mathrm{tr}((A^{-1})_i\tilde{X}^T)$, with $\tilde{X} = \begin{pmatrix} X & 0 \\ 0 & 0 \end{pmatrix}$, and the analogue for the other blocks. □

From condition 3 in the lemma above a very important equivalence can be easily derived: a 3-index tensor is injective if and only if the map associated to it as in eq. (19) is also injective. Indeed, this is why injective tensors are called like that.

5.1.4. Projectors associated to tensors. Let us now derive more relationships between tensors and their associated maps.

Definition 5.1.11 (Span of a tensor, Projector corresponding to a tensor). Given a tensor $(T_i)_{\alpha\beta}$ with two virtual indices α, β, and one physical index i (which can be a blocked index), we define the span of T as

$$\mathrm{span}\{T\} := \mathrm{span}\Big\{\sum_i \mathrm{tr}(T_i X)\,|i\rangle\,\Big|\,X \in \mathcal{M}_D\Big\}\ .$$

The span of a tensor T corresponds exactly to the range of the projection P in eq. (19) as introduced when defining the matrix product state formalism.

Also, we define the projector corresponding to T, $\Pi[T]$, as the orthogonal projector onto $\mathrm{span}\{T\}^\perp$.

In particular, T can arise from blocking two or more tensors A from a given MPS, $T = A\overset{c}{-}A\cdots$. E.g.,

$$\mathrm{span}\{A\overset{C}{-}A\} \equiv \mathrm{span}\Big\{\sum_{i,j}\mathrm{tr}(A_iA_jX)|i,j\rangle\Big|X \in \mathcal{M}_D\Big\}\ . \tag{23}$$

Lemma 5.1.12 (Gauge transformations for span). *Let $\mathcal{L}:\mathcal{M}_D \to \mathcal{M}_D$ be an invertible map on $D\times D$ matrices. Then,* $\mathrm{span}\{T\} = \mathrm{span}\{\mathcal{L}(T)\}$, *and equally* $\Pi[T] = \Pi[\mathcal{L}(T)]$, *where the natural action of $\mathcal{L}$ on three-index tensors $(T_i)_{\alpha\beta}$ is given by $[\mathcal{L}(T)]_i = \mathcal{L}(T_i)$.*

Proof.

$$\begin{aligned}\mathrm{span}\{\mathcal{L}(T)\} &= \mathrm{span}\Big\{\sum_i \mathrm{tr}(\mathcal{L}(T_i)X)\,|i\rangle\,\Big|\,X \in \mathcal{M}_D\Big\}\\ &= \mathrm{span}\Big\{\sum_i \mathrm{tr}(T_i(\mathcal{L}^*(X^*))^*)\,|i\rangle\,\Big|\,X \in \mathcal{M}_D\Big\}\\ &= \mathrm{span}\Big\{\sum_i \mathrm{tr}(T_iX)\,|i\rangle\,\Big|\,X \in \mathcal{M}_D\Big\}\\ &= \mathrm{span}\{T\}.\end{aligned}$$

□

Lemma 5.1.13 (Continuity of projector of a tensor). *Let $T(\varepsilon)$ be a family of tensors. If $T(0)$ is injective and $T(\varepsilon)$ is continuous around* 0*, then $\Pi[T(\varepsilon)]$ is continuous at* 0.

More generally, if $T(0)$ is block-injective and $T(\varepsilon)$ is continuous and block-diagonal in the same basis around 0*, then $\Pi[T(\varepsilon)]$ is continuous around* 0.

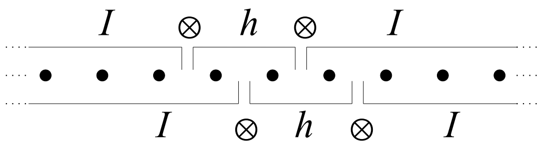
Proof. The proof follows directly from the fact that a basis X_k of the space of (block-)diagonal matrices yields a continuously changing basis of $\mathrm{span}\{T(\varepsilon)\}$ by virtue of $X_k \mapsto \sum_i \mathrm{tr}(T_i(\varepsilon)X_k)|i\rangle = |v_k(\varepsilon)\rangle$. From these bases, the Gram-Schmidt orthogonalization process leads also continuously to orthonormal changing bases of $\mathrm{span}\{T(\varepsilon)\}$, say $\{|e_k(\varepsilon)\rangle\}$. Note that injectivity of $T(0)$ implies maximal rank for the set $\{|v_k(0)\rangle\}_k$, and therefore injectivity of $T(0)$ and continuity of T at 0 is enough to ensure injectivity of

$T(\varepsilon)$ for small ε.

The final projection mapping $\varepsilon \mapsto \Pi[T(\varepsilon)]$ is also continuous, since projecting any vector onto the linear spaces $\operatorname{span}\{|e_k(\varepsilon)\rangle\}$ and substracting the result to the vector are continuous in ε.

In the case $T(0)$ is block-injective, the fact that $T(\varepsilon)$ is also block-diagonal makes the rank of $\{|v_k(\varepsilon)\rangle\}_k$ not grow and be constant around 0. This allows to guarantee the same result about continuity. Random perturbations would make the space $\operatorname{span}\{T(\varepsilon)\}$ much larger, and the variation of the projector would no longer be continuous. □

5.1.5. The parent Hamiltonian. Let us now turn towards Hamiltonians for MPSs. We will restrict to translationally invariant local Hamiltonians (i.e., defined as the sum of local terms representing local interactions), and denote the local terms by lowercase letters, e.g., h. When necessary, subscripts indicate the sites h acts on, e.g., $h_{i,i+1}$ when acting on two consecutive sites. We will identify the local operator h and the global operator $h \otimes \mathbb{I}$.



The global Hamiltonian will be denoted by the corresponding uppercase letter, e.g., $H = \sum h := \sum_{i=1}^{N} h_{i,i+1}$. Generally, indices will wrap around the ends of the chain (e.g., here $N + 1 \equiv 1$).

Every MPS $|M(A)\rangle$ induces Hamiltonians to which it is an exact ground state. If we focus on two consecutive sites – here we illustrate what happens with the first two sites – the MPS is described as

$$|M(A)\rangle = \sum_{i,j} \Big(\sum_{i_1,i_2} \langle i|A_{i_1}A_{i_2}|j\rangle |i_1 i_2\rangle \Big) \otimes \Big(\sum_{i_3,\dots,i_N} \langle j|A_{i_3}\cdots A_{i_N}|i\rangle |i_3\cdots i_N\rangle \Big) \Big).$$

Hence the reduced state on two adjacent sites is supported on $\operatorname{span}\{A \overset{c}{-} A\}$, and thus for $h := \Pi[A \overset{c}{-} A]$ we have $h|M(A)\rangle = 0$. If $D^2 < d^2$ – this can be achieved by blocking, and is the case for the standard form of Theorem 5.1.7 – $\Pi[A \overset{c}{-} A]$ is always non-trivial, and we obtain a non-trivial Hamiltonian with two-body terms h which has $|M(A)\rangle$ as ground state.

If we use $|M(A)\rangle$ in the standard form of Thm. 5.1.7, this Hamiltonian is particularly well-behaved:

Definition 5.1.14 (Parent Hamiltonian). Let $|M(A)\rangle$ be a (block-)injective MPS, i.e., satisfying condition 2 of Theorem 5.1.7 with every $\Gamma_j = 1$, and let $h = \Pi[A \overset{c}{-} A]$. Then, the Hamiltonian $H = \sum h$ is called the parent Hamiltonian.

Theorem 5.1.15 (Ground state space of parent Hamiltonian [**86, 101, 114**]). *The parent Hamiltonian has a $\mathcal{D}$-fold degenerate ground state space spanned by $|M(A^j)\rangle$; in particular, $|M(A)\rangle$ is one of its ground states – and it is the unique ground state if the MPS is injective. Also, the parent Hamiltonian is gapped in the thermodynamic limit.*

REMARKS 5.1.16. Note that in order to ensure the correct ground state subspace in Theorem 5.1.15, a weaker condition than the injectivity of each tensor used in Definition 5.1.14 is enough: It is sufficient to take projectors onto the orthogonal complement of the span of $k+1$ sites, where k is chosen such that blocking k sites makes the tensor injective [**112**].

We state here that parent Hamiltonians are gapped for completeness of the statement. A family of Hamiltonians is gapped if the energy gap corresponding to the difference between the lowest energy eigenvalue and the rest of spectral values is lower bounded by some uniform constant $\Delta > 0$ as the dimension of the system grows. We will further explain this notion and why it is important in another section.

We have also mentioned in some moments, and we will do in other sections, that the parent Hamiltonian is frustration free; this means that the ground states of the parent Hamiltonian are also ground states of each local interaction. That is, those states which minimize the energy of the system also minimize the energy locally. This fact is clear for the parent Hamiltonian, since the ground states are in the kernel of the global Hamiltonian and each local interaction, which are all positive.

5.2. Spectral gaps and thermodynamic limits.

As we already mentioned in Chapter 2, the different spectral values of a given observable[3] are the possible outcomes of the measurement of this observable. In the case of a Hamiltonian, these spectral values are the possible energy levels of the system. Related to these spectral values, the notion of gap of a given Hamiltonian is very important in Physics. It is directly related to the stability of the Hamiltonian against local physical perturbations, and it is crucial in the problem of classifying matter into phases.

Let us introduce the notion of spectral gap in this section, together with some of the tools used to deal with them. We will be referring to one-dimensional lattices or chains, but we will also need its generalization to two dimensional square lattices in the next chapter. All the definitions and results can be extended straightforward.

A given family of Hamiltonians acting respectively on finite chains – open or closed – of increasing length is said to be gapped if there exists a constant bound Δ between the lowest energy level or eigenvalue, corresponding to the ground state space, and the second lowest energy level, corresponding to lowest energy excitations. More notions of gap can be considered, mainly when there are a few low energy levels very close to each other which tend to have the same energy value as the dimension of the system grows – ground space splitting –, and which are separated at least a constant value Δ from higher energy levels.

[3]Actually, we explained in Chapter 2 the role of the eigenvalues when measuring observables in finite dimensional systems, but we said nothing about the rest of spectral values in the case of infinite dimensional systems. For the finite-dimensional case the whole spectrum is punctual, but when considering observables on infinite dimensional spaces the continuous spectrum may be non-empty. In this case, these spectral values can also be outcomes of the measurement, and the probability of the outcome to be in certain region is determined by the spectral measure E – Definition 5.2.12 and Theorem 5.2.13 – of that observable: when measuring on a state $|\varphi\rangle$, $P(\text{outcome } \in (a,b)) = \|E((a,b))(|\varphi\rangle)\|^2$.

We will need to avoid the fact that rescaling the Hamiltonians – depending on the chain length – might lead to vanishing gaps or, on the contrary, to increasing gaps, for which we will need a few technicalities. It will be convenient to define the Hamiltonian in terms of its local interactions.

For any subset Λ of a given finite chain L, we can consider the C^*-algebra of bounded operators acting on Λ as $\mathcal{U}(\Lambda) = \otimes_{x\in\Lambda}\mathcal{M}(\mathbb{C}^d)$, with d the physical dimension at every site. They are usually also called algebras of observables, since Hermitian operators span the whole algebra. They come together with natural inclusions

$$\begin{aligned} \mathcal{U}(\Lambda_1) &\hookrightarrow \mathcal{U}(\Lambda_2) \\ A &\mapsto A \otimes \mathbb{I}_{\Lambda_2\setminus\Lambda_1} \end{aligned} \tag{24}$$

whenever $\Lambda_1 \subset \Lambda_2$.

DEFINITION 5.2.1. An interaction is a map, defined on the subsets[4] of the lattice,

$$\Phi_L : \mathcal{P}(L) \to \mathcal{U}(L)$$

such that $\Phi(\Lambda) = \Phi(\Lambda)^*$ and $\Phi(\Lambda) \in \mathcal{U}(\Lambda)$ – considered into $\mathcal{U}(L)$ – for every $\Lambda \in \mathcal{P}(L)$.

The Hamiltonian is then defined as the sum of the interactions

$$H(|\varphi\rangle) = \sum_{\Lambda\subset L} \Phi(\Lambda)(|\varphi\rangle).$$

The translations $\tau_y(x) = x + y$ in the lattice induce translations into the algebra of operators, defined as $\tau_y(A_{(x)}) = A_{(x-y)}$ for an operator acting as A on site x and as the identity everywhere else, and extended by linearity to other operators. Translationally invariant interactions – $\Phi(\Lambda) = \tau_x(\Phi(\Lambda+x))$ – lead to translationally invariant Hamiltonians.

In the case of the parent Hamiltonian for an injective MPS described by an injective tensor A, which we previously described, the interaction would be a 2-body nearest-neighbour interaction defined on every lattice size as

$$\Phi(\Lambda) = \begin{cases} h_{\rm loc} = \Pi[A \stackrel{c}{-} A] & , \text{if } \Lambda = \{x, x+1\} \\ 0 & , \text{otherwise} \end{cases}.$$

In addition to translational invariance, we also require the interaction to be well-behaved under size growing. That is, for a given subchain Λ which can be included into two finite chains L_1 and L_2, we will have $\Phi_{L_1}(\Lambda) = \Phi_{L_2}(\Lambda)$, seen in $\mathcal{U}(\Lambda)$, whenever Λ involves no chain boundaries in either L_1 nor L_2 in the case of closed chains. This prevents wrong rescalings of Hamiltonians.

With all these requirements, the notion of Hamiltonian gap presented before makes complete sense. As an example, parent Hamiltonians show a spectral gap above the ground space level [**41, 86**]. Easier examples could be provided by commuting finite-range interactions – $[\Phi_L(\Lambda_1), \Phi_L(\Lambda_2)] = 0$ for every Λ_1, Λ_2, L, and $\Phi_L(\Lambda) = 0$ whenever $\mathrm{diam}(\Lambda) > k$ for some given fixed $k \in \mathbb{N}$.

However, sometimes one considers not only increasing chains, but an infinite chain. This lets us study the asymptotic behaviour of very long systems. Moreover, phase

[4]When considering infinite lattices, interactions will be defined onto the finite subsets of the lattice.

transitions must be studied in this framework, which is called the thermodynamic limit. For infinite chains a (bounded from below) thermodynamic limit Hamiltonian is said to be gapped if its lowest spectral value is isolated in the spectrum, and the dimension of the corresponding eigenspace leads to two different definitions of gap, depending on whether it is degenerate or not.

When trying to study systems on infinite chains, several problems arise. First of all, the infinite tensor product of even finite dimensional Hilbert spaces is no longer a separable Hilbert space. Two product states would be orthogonal unless they differ significantly in at most a finite number of sites, since for given $|\varphi\rangle = \otimes_{i=-\infty}^{\infty}|\varphi_i\rangle$ and $|\eta\rangle = \otimes_{i=-\infty}^{\infty}|\eta_i\rangle$ we have the inner product

$$\langle\varphi|\eta\rangle = \Pi_{i=-\infty}^{\infty}\langle\varphi_i|\eta_i\rangle.$$

In the second place, Hamiltonians turn generally to be unbounded operators, and notions as ground state may become ill-defined.

Let us next introduce some of the notions and tools needed to formalize thermodynamic limits.

5.2.1. Unbounded operators. First we will need to extend the usual definition of operator, so as to consider also linear maps which might be not defined on an entire Hilbert space but on a suitable subspace of it. Most of the following definitions and results can be found in [**32**], in the chapter devoted to spectral theory of unbounded operators.

DEFINITION 5.2.2. Let $\mathcal{H}$, $\mathcal{K}$ be Hilbert spaces. A linear operator – or just operator – is a linear map $A : \mathcal{H} \to \mathcal{K}$ such that it is defined on a linear subspace of $\mathcal{H}$: $\mathrm{dom}(A)$. As usual, such an operator is said to be bounded if there exists a constant k such that $\|Ax\| \le k\|x\|$, $\forall x \in \mathrm{dom}(A)$. We will consider operators such that $\mathrm{dom}(A)$ is dense in $\mathcal{H}$, which will be called densely defined operators.

Given two linear operators A and B from $\mathcal{H}$ to $\mathcal{K}$, $A + B$ is defined as the sum of A and B with domain $\mathrm{dom}(A + B) = \mathrm{dom}(A) \cap \mathrm{dom}(B)$. Given $A : \mathcal{H} \to \mathcal{K}$ and $B : \mathcal{K} \to \mathcal{L}$ two operators, BA is also an operator with domain $\mathrm{dom}(BA) = A^{-1}(\mathrm{dom}(B))$.

Given two linear operators $A, B : \mathcal{H} \to \mathcal{L}$, we say that B is an extension of A if $\mathrm{dom}(A) \subseteq \mathrm{dom}(B)$ and $B|_{\mathrm{dom}(A)} = A$. It will be denoted by $A \subseteq B$.

DEFINITION 5.2.3. Let $A : \mathcal{H} \to \mathcal{L}$ be an operator. The graph of A is the set

$$\{h \oplus A(h) \in \mathcal{H} \oplus \mathcal{L},\ h \in \mathrm{dom}(A)\}.$$

An operator $A : \mathcal{H} \to \mathcal{L}$ is said to be closed if its graph is a closed subset of $\mathcal{H} \oplus \mathcal{L}$. An operator is said to be closable if it has a closed extension, which happens whenever the closure of $\mathrm{graph}(A)$ in $\mathcal{H} \oplus \mathcal{L}$ is the graph of some function. Such function is, in this case, the closure of A.

Note that a densely defined bounded operator can be uniquely extended to a bounded operator on the entire Hilbert space $\mathcal{H}$, by considering its closure. Therefore, closed extensions will only make any significant difference in the case of unbounded operators. Closed extensions and closed operators will have a crucial role when studying self-adjoint unbounded operators. To this end, let us start with the definition of the adjoint for a given operator and some elementary results.

DEFINITION 5.2.4. Given a densely defined operator $A : \mathcal{H} \to \mathcal{L}$, the adjoint operator, A^*, is defined on the subspace

$$\text{dom}(A^*) = \{k \in \mathcal{L},\ h \mapsto \langle Ah|k\rangle \text{ is a bounded linear funcional on } \mathcal{H}\}.$$

Since $\text{dom}(A)$ is dense in $\mathcal{H}$, for every $k \in \text{dom}(A^*)$ there exists a unique element[5] $f_k \in \mathcal{H}$ such that $\langle Ah|k\rangle = \langle h|f_k\rangle$ for every $h \in \text{dom}(A)$. We define the image of k under A^* as $A^*k = f_k$, and therefore we have $\langle Ah|k\rangle = \langle h|A^*k\rangle$ for every $h \in \text{dom}(A)$, $k \in \text{dom}(A^*)$.

PROPOSITION 5.2.5. *Given a densely defined operator A,*

1. *A^* is a closed operator;*
2. *A^* is densely defined if and only if A is closable;*
3. *if A is closable, its closure is $(A^*)^*$.*

This takes us to the natural definition of self-adjoint operator.

DEFINITION 5.2.6. A densely defined operator $A : \mathcal{H} \to H$ is self-adjoint if $A = A^*$.

Note that in this last definition it is important that the domains of both A and A^* coincide. A self-adjoint operator verifies the usual requirement asked to bounded operators to be self-adjoint, that is, $\langle Ah|k\rangle = \langle h|Ak\rangle$ for every $k, h \in \mathcal{H}$. However, this is not enough in the case of unbounded operators. This condition on unbounded operators leads to the next definition.

DEFINITION 5.2.7. An operator $A : \mathcal{H} \to \mathcal{H}$ is symmetric if it is densely defined and $\langle Ah|k\rangle = \langle h|Ak\rangle$ for every $k, h \in \mathcal{H}$.

Moment operator from Quantum Mechanics – $Af = \frac{-i}{\hbar} f'$ – provides one of the typical examples of symmetric operators which may be not self-adjoint, depending on the domain it is defined on.

Symmetric operators may have very strange properties. Among others, they may have many different self-adjoint extensions. We will be especially interested in the case in which they have just one self-adjoint extension, which will be identified using what are called analytic elements.

DEFINITION 5.2.8. A symmetric operator is said to be essentially self-adjoint if it has a unique self-adjoint extension. In particular, its closure must be this unique self-adjoint extension.

DEFINITION 5.2.9. A vector $|\varphi\rangle$ is analytic for a given operator A if $|\varphi\rangle \in \text{dom}(A^n)$ for every $n \in \mathbb{N}$, and there exists some $r > 0$ such that

$$\sum_{n=0}^{\infty} \frac{r^n}{n!} \|A^n(|\varphi\rangle)\| < \infty.$$

PROPOSITION 5.2.10. **[120]** *A symmetric operator $A : \mathcal{H} \to \mathcal{H}$ is essentially self-adjoint if it has a set of analylitic elements which is dense in $\mathcal{H}$.*

Analytic elements essentialy ensure that $e^{\lambda A}$ can be defined for them at least at some radius around 0. We will find these elements important at two points, when defining groups of automorphisms from an unbounded derivation, and when studying essentially selfadjointness of the symmetric operator which will evidence the candidate to be a

[5]Due to Riesz Representation Theorem.

Hamiltonian.

The subtleties regarding the domain of unbounded operators introduce a minor change in the requirements for an element $\lambda \in \mathbb{C}$ to be in the resolvent set of a given operator, since densely defined unbounded operators cannot have a proper left inverse whenever its domain is not the whole space.

Definition 5.2.11. Let $A : \mathcal{H} \to \mathcal{H}$ be a linear operator. A is boundedly invertible if there exists a bounded operator B such that $AB = \mathbb{I}$ and $BA \subseteq \mathbb{I}$.

An element $\lambda \in \mathbb{C}$ is said to be in the resolvent set of A if $A - \lambda\mathbb{I}$ is boundedly invertible. The spectrum of A is the complement of the resolvent set in $\mathbb{C}$.

The resolvent set is open in $\mathbb{C}$, and consequently the spectrum is closed. For closed unbounded operators, we have the same disjoint decomposition of the spectrum into its point, continuous and residual parts[6] as we have for bounded operators. For non-closed operators, we have that the spectrum is the entire field $\mathbb{C}$.

We will study the spectra of unbounded Hamiltonians, which are unbounded self-adjoint operators, and we will take advantage of the fact that the residual spectrum of any self-adjoint unbounded operator is empty and its spectrum must be real.

These Hamiltonians will also be positive, that is, self-adjoint operators A for which $\langle Ax|x\rangle \geq 0$ for every x in $\mathrm{dom}(A)$. In this case, $\sigma(A) \subseteq \mathbb{R}^+$.

We will also use the spectral theorem, either for bounded or for unbounded normal operators, depending on the case.

Definition 5.2.12. If X is a set, Ω is a σ-algebra of subsets of X, and $\mathcal{H}$ is a Hilbert space, a spectral measure for $(X, \Omega, \mathcal{H})$ is a function $E : \Omega \to B(\mathcal{H})$ such that:

a) for each Δ in Ω, $E(\Delta)$ is a projection;

b) $E(\varnothing) = 0$ and $E(X) = \mathbb{I}$;

c) $E(\Delta_1 \cap \Delta_2) = E(\Delta_1)E(\Delta_2)$ for $\Delta_1, \Delta_2 \in \Omega$ (and therefore every pair of such projectors commute, since intersection of sets is commutative);

d) if $\{\Delta_n\}_{n=1}^{\infty}$ are pairwise disjoint sets from Ω, then $E(\bigcup_{n=1}^{\infty} \Delta_n) = \sum_{n=1}^{\infty} E(\Delta_n)$.[7]

Theorem 5.2.13 (Spectral Theorem for normal bounded and unbounded operators). *If N is a normal operator on $\mathcal{H}$, then there is a unique spectral measure E defined on the Borel subsets of $\sigma(N)$ such that:*

a) $N = \int_{\sigma(N)} z dE(z)$,

b) if U is an nonempty open subset of $\sigma(N)$, then $E(U) \neq 0$.

5.2.2. Heisenberg picture, observables dynamics and equilibrium states. The importance of the Hamiltonian in Quantum Mecanichs stems on the fact that it

[6]A value $\lambda \in \mathbb{C}$ is in the point spectrum of A if $A - \lambda\mathbb{I}$ is not injective, in the continuous spectrum if $A - \lambda\mathbb{I}$ has an inverse which is densely defined but not bounded – and therefore $AB \subset \mathbb{I}$ – and in the residual spectrum if $A - \lambda\mathbb{I}$ is injective on $\mathrm{dom}(A)$ but has non-dense image.

[7]Considering convergence in the strong operator topology.

governs the dynamics of the systems, via the Schrödinger equation

$$\frac{d}{dt}|\varphi(t)\rangle = -iH(t)|\varphi(t)\rangle,$$

where the reduced Planck's constant $\hbar$ is considered as part of the Hamiltonian operator H.

Let us first describe how this evolution is for finite dymensional systems, which we will generalize later for infinite dimensional systems. Most of the mathematical contents in this subsection and next subsection, such as KMS-states and ground states in the Heisenberg picture, GNS-representation, and the theorems we use, can be found in [**20**].

For time-independent Hamiltonians on finite dimensional systems, we have as a result of the Schrödinger equation unitary time evolutions

$$|\varphi(t)\rangle = U_t|\varphi(0)\rangle,$$

with $U_t = e^{-itH}$. Stone's Theorem guarantees the converse relation: for every strongly continuous[8] semigroup of unitaries U_t acting on a Hilbert space such that $U_0 = \mathbb{I}$, there exists a unique self-adjoint operator H such that $U_t = e^{itH}$. The operator iH is the infinitesimal generator of the semigroup U_t.

Under this conditions, the expected result of measuring a given observable A would be

$$\langle\varphi(t)|A|\varphi(t)\rangle = \langle\varphi|U_t^* A U_t|\varphi\rangle = \langle\varphi|e^{itH}Ae^{-itH}|\varphi\rangle$$

for a given initial pure state $|\varphi\rangle$, and

$$\mathrm{tr}(e^{itH}Ae^{-itH}\rho)$$

for a given initial mixed state ρ.

Now one can think that the state – either pure of mixed – remains fixed, and the time evolution is affecting to the observables. This is called the Heisenberg picture, in opposition to the Schrödinger picture, which is the one we described before.

In this setting, one can see the states as linear functionals on the C^*-algebra of observables $\mathcal{U}(L)$ for a finite lattice L, resulting to have the same properties usually states are required in C^*-algebra theory. States are linear functionals

$$\omega : \mathcal{U}(L) \to \mathbb{C},$$

such that $\omega(\mathbb{I}) = 1$ and $\omega(A^*A) \geq 0$ for any A[9]. Any state ρ as defined in Chapter 2 – positive density matrices ρ with $\mathrm{tr}(\rho) = 1$ – induces a state on the C^*-algebra of observables ω_ρ, defined as $\omega_\rho(A) = \mathrm{tr}(A\rho)$. The former distinction between pure and mixed states corresponds to the distinction between extremal an non-extremal states as functionals.

[8] $\|U_t - U_{t_0}\| \to 0$ when $t \to t_0$. For finite-dimensional systems, weakly continuous and strongly continuous are equivalent.

[9] For C^*-algebras without identity, which is not our case, instead of $\omega(\mathbb{I}) = 1$ the requirement for a positive linear functional to be a state is $\|\omega\| = 1$. Note that the positivity condition on the functionals – $\omega(A^*A) \geq 0$ for any A – implies their cointinuity.

In this dual picture, unitary evolutions can be translated into semigroups of automorphisms of the C^*-algebra

$$\alpha_t : \mathcal{U}(L) \to \mathcal{U}(L), \ \alpha_t(A) = U_t^* A U_t.$$

And any strongly continuous semigroup of automorphisms of the C^*-algebra is determined, up to a phase, by a unitary evolution of this type. Consequently, there exists a unique self-adjoint operator H, up to an additive constant $\mu\mathbb{I}$, which induces this automorphisms as its Hamiltonian. Note that this freedom in the choice of the Hamiltonian has no effect in the spectral gap, nor in which states are ground states.

Another element we will use is symmetric derivations. Symmetric derivations, or just derivations in the following, are linear maps

$$\delta : \mathcal{U}(L) \to \mathcal{U}(L)$$

such that $\delta(AB) = A\delta(B) + \delta(A)B$ and $\delta(A^*) = \delta(A)^*$. They are the infinitesimal generators of such semigroups of automorphisms, and can be calculated from them as

$$\delta(A) = \left.\frac{d}{dt}\right|_{t=0} \alpha_t(A).$$

For a semigroup of automorphisms induced by a given Hamiltonian H, the derivation is $\delta(A) = i[H, A]$. For a given derivation δ, the corresponding automorphisms are

$$\alpha_t(A) = e^{t\delta}(A) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \delta^n(A).$$

Under these time evolutions, every eigenstate of the Hamiltonian will remain unchanged up to a phase. Let $|\varphi_\lambda\rangle$ be an eigenstate for an eigenvalue λ of H, then $e^{-itH}|\varphi_\lambda\rangle = e^{-it\lambda}|\varphi_\lambda\rangle$. Therefore, for $U_t = e^{-itH}$, we have $U_t^* \rho U_t = \rho$, for any ensemble of eigenstates ρ.

Among all these ensembles there is a distinguised family, the so-called thermal states or Gibbs states. These states are those states which remain in equilibrium when the system is coupled to a thermal bath. For a given temperature T, the corresponding Gibbs state is

$$\rho_\beta = \frac{e^{-\beta H}}{\mathrm{tr}(e^{-\beta H})},$$

where the parameter β is the inverse of the temperature – $\beta = 1/T$. From this family, the ground states can be recovered by letting β tend to infinity. Whenever the Hamiltonian has a unique ground state, the limit will be the projector onto it. And in the case the ground space is degenerate – the dimension of the ground state space is bigger than 1 – the limit will be proportional to the projector onto the ground state space.

When considering the equivalent to thermal states in the Heisenberg picture, the condition they fulfill is the KMS-condition[10]:

$$\omega\left(\alpha_t(A)B\right) = \omega\left(B\alpha_{t+i\beta}(A)\right), \forall A, B \in \mathcal{U}(L).$$

States verifying KMS-conditions are called KMS-states. By letting β tend to infinity we get the condition for a state ω to be a ground state for the evolution α_t:

$$-i\omega\left(A^*\delta(A)\right) \geq 0, \ \forall A \in \mathcal{U}(L).$$

[10]Named after Kubo, Martin and Schwinger.

These two conditions will be well-defined for infinite lattices, and will be our starting point in order to find the limit Hamiltonian for infinite systems.

Even though the ground state condition might look strange at first sight, it is not only the limit at zero temperature of the KMS-condition, but also the one which characterizes some mean energy[11] minimization condition, which will also be transferred properly to infinite lattices. To this end let us consider the mean energy associated to a translationally invariant interaction Φ and a translationally invariant state ω by

$$H_\Phi(\omega) = \sum_{a\in\Lambda} \frac{\omega(\Phi(\Lambda))}{|\Lambda|}.$$

Note that the element a in the lattice makes no difference due to translational invariance of both interaction and state.

5.2.3. The thermodynamic limit. When letting the system size grow up to infinity, even though we cannot directly deal with a limit Hilbert space, we can construct the algebra of observables and the dynamics on it in the Heisenberg picture, and we can extend the concept of KMS-state and ground state.

From now on, the lattice of the system will be $L = \mathbb{Z}$ in the one-dimensional case. And the C^*-algebra will be the algebra of quasi-local observables, $\mathcal{U}_{\text{loc}}(L)$, which is the direct limit of the C^*-algebras $\mathcal{U}(\Lambda)$ for $\Lambda \in \mathcal{P}_f(L)$, where $\mathcal{P}_f(L)$ denotes the set of finite subsets of L, with the inclusions described in (24). This is the norm completion of

$$\bigcup_{\Lambda\in\mathcal{P}_f(L)} \mathcal{U}(\Lambda).$$

Given an interaction Φ on the lattice, we start by considering the Hamiltonian acting on a finite region Λ – with open boundary conditions – defined by $H_\Lambda = \sum_{\bar\Lambda\subseteq\Lambda} \Phi(\bar\Lambda)$. This Hamiltonian induces a semigroup of automorphisms on $\mathcal{U}_{\text{loc}}(L)$ which determines the corresponding dynamics on the observables:

$$\alpha_t^\Lambda(A) = e^{itH_\Lambda} A e^{-itH_\Lambda}.$$

In order to see that the automorphisms α_t^Λ certainly converge when Λ tends to be the whole lattice, one makes use of the derivations

$$\delta_\Lambda = i[H_\Lambda, A].$$

Let us consider the derivation defined as the limit

$$\delta(A) = \lim_{\Lambda\to L} \delta_\Lambda(A),$$

whenever this limit exists. For finite-range interactions, which will be our case, this derivation is, at least, densely defined on $\mathcal{U}_{\text{loc}}(L)$, for it is well defined on every subalgebra $\mathcal{U}(\Lambda)$, $\Lambda \in \mathcal{P}_f(L)$.

This derivation has a dense set of analytic elements, since every observable in any $\mathcal{U}(\Lambda)$, with Λ finite, is analytic for δ. This let us state that $\alpha_t = e^{t\delta}$ is also densely defined, and, since it is bounded, can be uniquely extended to an automorphism of the whole algebra of quasi-local observables for every t.

[11]In this paragraph mean energy refers to average energy per site.

The only elements we are lacking now are the Hilbert space and the Hamiltonian. In the previous finite dimensional setting the algebra of observables was already acting in a Hilbert space, but in this case we need to fix a given state – a ground state will be the right choice – and take the corresponding GNS-representation to be able to capture this dynamics.

DEFINITION 5.2.14. A representation of a C^*-algebra $\mathcal{U}$ is a pair $(\mathcal{H}, \pi)$, where $\mathcal{H}$ is a Hilbert space and π is a $*$-homomorphism of $\mathcal{U}$ into $\mathcal{L}(\mathcal{H})$.

A cyclic representation of a C^*-algebra $\mathcal{U}$ is a triple $(\mathcal{H}, \pi, \Omega)$, such that $(\mathcal{H}, \pi)$ is a representation of $\mathcal{U}$, and Ω is a vector in $\mathcal{H}$ – called also cyclic in this case – such that $\pi(\mathcal{U})\Omega$ is dense in $\mathcal{H}$.

THEOREM 5.2.15 (Gelfand-Neimark-Segal Representation). *Given a C^*-algebra $\mathcal{U}$ with identity and a state ω on it, there exists a essentialy unique, up to unitary equivalence, cyclic*[12] *representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ such that $\omega(A) = \langle \Omega_\omega | \pi_\omega(A)\Omega_\omega \rangle$ for all $A \in \mathcal{U}$. Consequently, $\|\Omega_\omega\|^2 = \|\omega\| = 1$.*

In order to construct the GNS-representation, one first considers in $\mathcal{U}$ the possibly degenerate inner product induced by ω,

$$\begin{aligned} (\cdot,\cdot) : \mathcal{U} \times \mathcal{U} &\to \mathbb{C} \\ (A, B) &\mapsto \omega(A^*B) \end{aligned}$$

The second step is to consider the closed left ideal $\mathcal{I} = \{A, \omega(A^*A) = 0\}$, and take the quotient $\mathcal{U}/\mathcal{I}$, which is a preHilbert space with the inner product induced by the possibly degenerate one previously considered. Let us call ξ_A the class corresponding to an element A of $\mathcal{U}$.

The Hilbert space $\mathcal{H}_\omega$ of the representation is the completion of this last preHilbert space.

The representation we take is

$$\begin{aligned} \pi_\omega(A) : &\mathcal{H}_\omega \to \mathcal{H}_\omega \\ &\xi_B \mapsto \xi_{AB}. \end{aligned}$$

which is bounded and densely defined for every $A \in \mathcal{U}$, and therefore has a bounded closure, also called $\pi_\omega(A)$. We take as distinguished cyclic vector $\Omega_\omega = \xi_{\mathbb{I}}$.

With this representation, one can finally get the set of unitaries which determines the evolution and the associated Hamiltonian.

THEOREM 5.2.16. Let ω be a state over a C^*-algebra $\mathcal{U}$ and α_t an automorphism semigroup of it which leaves ω invariant – $\omega(\alpha_t(A)) = \omega(A)$ for all $A \in \mathcal{U}$. Then there exists a uniquely determined strongly continuous semigroup of unitary operators $U_{\omega,t}$ on the space of the GNS-representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ constructed from ω such that

$$U_{\omega,t}^* \pi_\omega(A) U_{\omega,t} = \pi_\omega(\alpha_t(A))$$

[12]A representation $(\mathcal{H}, \pi, e)$ of a C^*-algebra $\mathcal{U}$ is called cyclic if $\pi(U)e$ is dense in $\mathcal{H}$. Such vector e is also called cyclic.

for all $A \in \mathcal{U}$ and all t, and

$$U_{\omega,t}\Omega_\omega = \Omega_\omega$$

for all t.

This family of unitaries corresponds[13] to a uniquely determined self-adjoint Hamiltonian H_ω such that $U_{\omega,t} = e^{itH_\omega}$, and one has that it is positive if ω is a ground state for α_t.

THEOREM 5.2.17. Given $\mathcal{U}(L)$ and α_t as before, the following are equivalent:

(1) ω is a ground state for α_t;
(2) ω is α_t-invariant, and the Hamiltonian H_ω, resulting from the construction of the GNS-representation with respect to ω as described above, is positive.

And, moreover, for a finite-range translationally invariant interaction Φ and a translationally invariant state ω, ω is a ground state with respect to the evolution determined by Φ if and only if ω minimizes the mean local energy H_Φ.

The positive Hamiltonian H_ω is considered as the effective Hamiltonian to study. Note that it depends on the ground state considered, hence its spectral properties might differ depending on the ground state it is constructed from. Note also that the property $U_{\omega,t}\Omega_\omega = \Omega_\omega$ for all t in Theorem 5.2.16 implies $H_\omega\Omega_\omega = 0$, and therefore $0 \in \sigma(H)$ is the lowest spectral value. A thermodynamic limit Hamiltonian H_ω is said to be gapless if 0 is not an isolated value of its spectrum.

Phisically, the Hilbert space $\mathcal{H}_\omega$ can be seen as the possible configurations with finite energy which come from excitations of a given ground state ω. Every finite energy configuration must come from one ground state.

5.3. Uncle Hamiltonians: definition and toy example.

Let us now study the problem of the non-robustness of the parent Hamiltonian construction, which we first detail for the GHZ state.

5.3.1. The uncle Hamiltonian. The parent Hamiltonian construction can be interpreted as a map from the set of MPS to the set of Hamiltonians, $\hat{H} : A \mapsto \hat{H}(A)$, which associates to any MPS $|M(A)\rangle$ its parent Hamiltonian $\hat{H}(A)$. While this map is well-behaved in terms of the properties of $\hat{H}(A)$, we are also interested in its continuity: If we change A smoothly, $A \to A + \varepsilon P$, does $\hat{H}(A)$ change smoothly as well? Were this the case, this would allow us to study perturbations of the system by looking at perturbations of the MPS tensor A. For injective MPS in their standard form, Lemma 5.1.13 tells us that this is indeed the case. On the other hand, if A is block-injective, Lemma 5.1.13 requires P to be block-diagonal as well, and it is indeed easy to see that *random* perturbations P will lead to a discontinuous change in $\hat{H}(A + \varepsilon P)$, as $\dim(\operatorname{span}\{(A + \varepsilon P) \overset{c}{-} (A + \varepsilon P)\})$ may increase in this case when ε changes from 0 to nonzero values.

This discontinuity motivates the introduction of the uncle Hamiltonians, which are robust under specific perturbations of the MPS tensor.

[13]Stone's Theorem also apply to the infinite dimensional setting, leading to possibly unbounded Hamiltonians.

Definition 5.3.1 (Uncle Hamiltonians). Let $|M(A)\rangle$ be an MPS in standard form, and let $\{P_i\} \subset \mathcal{M}_D$ with the same number of matrices as A. Then, the uncle Hamiltonian induced by P is the Hamiltonian

$$H'_P := \lim_{\varepsilon \to 0} \hat{H}(A + \varepsilon P) \ , \tag{25}$$

whenever this limit exists. This is, the uncle Hamiltonian is the limit of the parent Hamiltonian for the perturbed MPS for the perturbation going to zero.

As well as $\hat{H}$ is the sum of local Hamiltonians, so is H'_P. Each local term of the uncle Hamiltonian, which we call h'_P, is the limit as ε vanishes of the corresponding local term of the parent Hamiltonians $\hat{H}(A + \varepsilon P)$. Therefore

$$h'_P := \lim_{\varepsilon \to 0} \Pi[(A + \varepsilon P) \overset{C}{—} (A + \varepsilon P)],$$

and the uncle Hamiltonian can be expressed as $H'_P = \sum h'_P$.

As we mentioned, for A an injective tensor this limit exists and is equal to the local term of the parent Hamiltonian, following Lemma 5.1.13. Therefore, parent and uncle Hamiltonian coincide for injective MPS. Thus, we focus our attention on the uncle Hamiltonians for block-injective MPS. Next diagram summarizes the construction for block-injective MPSs, where $h = \Pi[A \overset{C}{—} A]$ denotes the local term of the parent Hamiltonian for A, and $h^\varepsilon = \Pi[(A + \varepsilon P) \overset{C}{—} (A + \varepsilon P)]$ denotes the local term of the parent Hamiltonian for the corresponding perturbed tensor.

In the following, $H = \sum h$ will denote the parent Hamiltonian, and we will occassionally omit the subscript P when referring to the uncle Hamiltonian $H'_P = \sum h'_P$.

5.3.2. Toy example: uncle Hamiltonian for the GHZ state. We start our discussion on the properties of the uncle Hamiltonian with the GHZ state . As we already mentioned when introducing the definition of the Matrix Product States, the unnormalized GHZ state can be expressed as an MPS as

$$|\mathrm{GHZ}\rangle = |00\cdots 0\rangle + |11\cdots 1\rangle = \sum_{i_1,\ldots,i_L} \mathrm{tr}(A_{i_1} \ldots A_{i_L}) |i_1, \ldots, i_L\rangle$$

with $i_j \in \{0,1\}$, where $A_0 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ and $A_1 = \left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right)$. Following Definition 5.1.14, the parent Hamiltonian for the GHZ state can be constructed from the span of two sites,

$$\mathrm{span}\{A \overset{C}{—} A\} = \mathrm{span}\{|00\rangle, |11\rangle\} \ ,$$

which is indeed (up to an additive constant) the well-known Ising Hamiltonian

$$\tfrac{1}{2}\mathbb{I} - \big[|00\rangle\langle 00| + |11\rangle\langle 11|\big].$$

Let us now construct the uncle Hamiltonian for the GHZ state. According to the definition, we first need to fix a perturbation P of the MPS tensor A:

$$P_0 = \begin{pmatrix} a_0 & b_0 \\ c_0 & d_0 \end{pmatrix} \quad \text{and} \quad P_1 = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \ . \tag{26}$$

Next, we need to consider the MPS associated to the perturbation, which is $|M(C_{\varepsilon,P})\rangle$ for $C_{\varepsilon,P} = A + \varepsilon P$, and construct its parent Hamiltonian. For a generic P, we need to block two sites to reach injectivity. Thus, following Remark 5.1.16, we need to construct the terms of the parent Hamiltonian as the projector onto the complement of the span on three sites,

$$\mathcal{S}_3(\varepsilon) = \mathrm{span}\{C_{\varepsilon,P} \overset{c}{-} C_{\varepsilon,P} \overset{c}{-} C_{\varepsilon,P}\} \ .$$

$S_3(\varepsilon)$ is spanned by the four vectors $v_{\alpha\beta} = \langle\alpha|C_{\varepsilon,P} \overset{c}{-} C_{\varepsilon,P} \overset{c}{-} C_{\varepsilon,P}|\beta\rangle$, $\alpha,\beta = 0,1$, which are straightforwardly found to be

$$\begin{aligned}
v_{00} &= |000\rangle + O(\varepsilon) \ , \\
v_{01} &= \varepsilon\big[b_0|000\rangle + (b_0+b_1)|001\rangle + (b_0+b_1)|011\rangle + b_1|111\rangle\big] + O(\varepsilon^2) \ , \\
v_{10} &= \varepsilon\big[c_0|000\rangle + (c_0+c_1)|100\rangle + (c_0+c_1)|110\rangle + c_1|111\rangle\big] + O(\varepsilon^2) \ ; \\
v_{11} &= |111\rangle + O(\varepsilon) \ .
\end{aligned}$$

If $b_0 + b_1 \neq 0$ and $c_0 + c_1 \neq 0$ (which happens almost surely[14]), this can be transformed into an alternative set spanning $S_3(\varepsilon)$,

$$\big\{|000\rangle + O(\varepsilon), |001\rangle + |011\rangle + O(\varepsilon), |100\rangle + |110\rangle + O(\varepsilon), |111\rangle + O(\varepsilon)\big\} \ . \tag{27}$$

The parent Hamiltonian for the perturbed MPS $|M(C_{\varepsilon,P})\rangle$ is thus $H_{P,\varepsilon} = \sum h_{P,\varepsilon}$, with each $h_{P,\varepsilon}$ acting locally on three consecutive sites, and projecting onto $S_3(\varepsilon)^\perp$.

In order to obtain the uncle Hamiltonian we finally need to take the limit $\varepsilon \to 0$. Then, the four states in eq. (27) become orthogonal, and the family $h_{P,\varepsilon}$ converges to the projection onto the orthogonal complement of

$$\mathrm{span}\{|000\rangle, |0{+}1\rangle, |1{+}0\rangle, |111\rangle\}.$$

Here, $|0{+}1\rangle \equiv |0\rangle|{+}\rangle|1\rangle$, with $|{+}\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Thus, the uncle Hamiltonian has local terms

$$h'_P = \mathbb{I} - \big(|000\rangle\langle 000| + |111\rangle\langle 111| + |0{+}1\rangle\langle 0{+}1| + |1{+}0\rangle\langle 1{+}0|\big) \tag{28}$$

Note that this limit does not depend on the perturbation P (as long as $b_0 + b_1 \neq 0$ and $c_0 + c_1 \neq 0$), and will be called h' in the following, or $h'_{i-1,i,i+1}$ whenever we need to make it explicit which sites it is acting on. The uncle Hamiltonian H' is obtained as the sum

$$H' = \sum h' \equiv \sum_i h'_{i-1,i,i+1}.$$

5.3.3. Ground space of the uncle Hamiltonian for the GHZ state. We wonder first what is the ground space of the uncle Hamiltonian. Since

$$\ker(h') = \mathrm{span}\{|000\rangle, |111\rangle, |0+1\rangle, |1+0\rangle\} \supset \mathrm{span}\{|000\rangle, |111\rangle\} = \ker h \ ,$$

the ground states $|0\ldots 0\rangle$ and $|1\ldots 1\rangle$ which span the ground state space of the GHZ parent Hamiltonian are also ground states of the uncle; in particular, the uncle is also frustration free. However, h' allows for additional ground states. Indeed, if we consider the ground state space of h' acting on m consecutive sites (with open boundaries), the ground space is

$$\mathrm{span}\Big\{|0\ldots 0\rangle, |1\ldots 1\rangle, \sum_{\mathrm{pos}\, i=1}^{m-1} |0\cdots 0^i 1\cdots 1\rangle, \sum_{\mathrm{pos}\, i=1}^{m-1} |1\cdots 1^i 0\cdots 0\rangle\Big\} \subseteq (\mathbb{C}^2)^{\otimes m},$$

[14]Note that whenever we say something happens almost surely means not only that it happens with probability 1 but also that the set of perturbations which may not satisfy the statement forms a closed algebraic variety of dimension strictly lower than the set of all possible perturbations

where the sums run over all positions of the 'boundary wall' 01 and 10 respectively, and the superscript indicates the position of the corresponding qubit. (This notation will be used throughout this chapter and the next chapter.)

Yet, when closing the boundaries and considering periodic conditions, the additional states $\sum_{\mathrm{pos}\, i} |0\cdots0^i1\cdots1\rangle$ and $\sum_{\mathrm{pos}\, i} |1\cdots1^i0\cdots0\rangle$ stop being in the intersection of the kernels. Intuitively, with periodic boundary conditions the boundary walls need to come in pairs. Hence the ground space of the uncle Hamiltonian coincides with the ground space of the parent Hamiltonian.

5.3.4. Spectrum of the uncle Hamiltonian for the GHZ state. The spectra of parent Hamiltonians show a spectral gap over the ground state level. On the contrary, uncle Hamiltonians are generally gapless, as we shall prove later. This example we are studying now is no exception to this different behaviour.

Let us first show that the uncle Hamiltonian for the GHZ state is not gapped when considered as acting on finite chains. To this end, we consider the unnormalized states

$$|\phi_N\rangle = \sum_{\substack{-N\le i\le -1\\ 1\le j\le N}} |\phi_{i,j}\rangle \tag{29}$$

with

$$|\phi_{i,j}\rangle = |0^{-N-1}0\cdots0^i1\cdots10^j\cdots0^{N+1}\rangle$$

on a chain of length $2N+3$.

These states are orthogonal to the ground space, and $\langle\phi_N|\phi_N\rangle = N^2$. They are ground states of all local terms in H' except $h'_{-1,0,1}$, $h'_{N,N+1,-N-1}$, and $h'_{N+1,-N-1,-N}$, and by counting the violating[15] configurations, we find that $\langle\phi_N|H'|\phi_N\rangle = O(N)$. Hence, for the energies of these states we have

$$\frac{\langle\phi_N|H'|\phi_N\rangle}{\langle\phi_N|\phi_N\rangle} = O(1/N).$$

Since these states are orthogonal to the ground space, this implies that (on a chain of length $2N+3$) H' has at least one eigenvalue $\lambda_N \le \frac{\langle\varphi_N|H'|\varphi_N\rangle}{\langle\varphi_N|\varphi_N\rangle} = O(1/N)$, i.e., the family of uncle Hamiltonians is gapless.

Unfortunately, the existence of states with energy $O(1/N)$ does not allow to conclude more properties about the spectrum of H': The existence of a state with energy E only implies the existence of eigenvalues $\lambda_1 \le E$ and $\lambda_2 \ge E$ – possibly the same –, but tells us nothing about their exact value.

In order to study more properties of the spectra of the uncle Hamiltonians we move to the study of the thermodynamic limit. We will treat this example informally. The detailed and formal treatment for generic MPSs can be found in Section 5.4.4. The spectrum in the thermodynamic limit can be found to be the whole positive real line and the spectra of the finite sized chains can be proven to tend to be dense in the positive real line. This can be shown by mapping this uncle Hamiltonian to the well-known XY model, as we do in Section 5.3.6. However, we detail here an alternative proof which illustrates the process we will need to follow later when considering generic non-injective MPSs.

[15]We say there is a violation whenever a local Hamiltonian does not vanish on a given state.

Through the GNS-representation the problem is translated in the GHZ case into studying the action of H' on the completion of the space

$$S = \bigcup_{i\le j\in\mathbb{Z}} S_{i,j}, \text{where } S_{i,j} = (\otimes_{n=-\infty}^{i-1}|0\rangle) \otimes (\otimes_{n=i}^{j}\mathbb{C}^2) \otimes (\otimes_{n=j+1}^{\infty}|0\rangle),$$

denoted by $\bar{S}$, and the spectrum of its unique self-adjoint extension $H'_\omega : \bar{S} \longrightarrow \bar{S}$. ω can be seen as the state induced by $|\cdots 0000\cdots\rangle\langle\cdots 0000\cdots|$ in this setting.

In order to prove that the thermodynamic limit of the uncle Hamiltonian is gapless we consider the uncle Hamiltonian restricted to the closure of the subspace

$$S^1 = \operatorname{span}\{e_{i,j} = |\cdots 00\cdots 0^i 11\cdots 1^j 0\cdots 0\cdots\rangle,\ i<j\}.$$

First we check that $H'_{\omega|_{S^1}}$ is bounded (Lemma 5.3.2). Consequently, it can be uniquely extended to a bounded self-adjoint operator defined on $\overline{S^1}$, which is $H'_\omega|_{\overline{S^1}}$ and will be called H''_ω.

This allows us to use the Spectral Theorem for normal bounded operators, together with low energy states similar to those described before, to prove that this operator is also gapless (Proposition 5.3.3). Therefore, there exists a sequence of elements $\{\lambda_n\}$ in the spectrum of this operator which tends to 0.

This last fact, together with the additive local structure of H', will let us compute the spectrum of H'_ω (Theorem 5.3.7).

LEMMA 5.3.2. *$H'_\omega(S^1) \subseteq S^1$ and $H'_\omega|_{S^1}$ is bounded.*

PROOF. We first check that $H'_\omega(e_{i,j}) \in S^1$, $i<j$. For any $e_{i,j}$, at most four local Hamiltonians do not vanish: $h'_{i-1,i,i+1}$, $h'_{i,i+1,i+2}$, $h'_{j-1,j,j+1}$ and $h'_{j,j+1,j+2}$.

If $i<j-1$ then none of these local Hamiltonians coincide, and

$$H'_\omega(e_{i,j}) = e_{i,j} - (e_{i-1,j} + e_{i+1,j} + e_{i,j-1} + e_{i,j+1})/2.$$

In the case $i = j-1$ we have that $H'_\omega(e_{i,j}) = 2e_{i,j} - (e_{i-1,j} + e_{i,j+1})/2$.

In either case $H'_\omega(e_{i,j}) \in S^1$, and we have therefore proven the first part of the result.

To check that the restriction of H'_ω to S^1 is bounded, let us take an element a from S^1. a can be expressed in term of the basis $\{e_{i,j}, i<j\}$ as $a = \sum_{i<j}\alpha_{i,j}e_{i,j}$, with the coefficients in ℓ_2.

We have then that

$$\begin{aligned}\|H'_\omega(a)\| =& \|\sum_{i<j-1}\alpha_{i,j}(e_{i,j} - (e_{i-1,j} + e_{i+1,j} + e_{i,j-1} + e_{i,j+1})/2) + \\ &+ \sum_i \alpha_{i,i+1}(2e_{i,i+1} - (e_{i-1,i+1} + e_{i,i+2})/2)\| \le \\ \le& \|\sum_i \alpha_{i,i+1}2e_{i,i+1} + \sum_{i<j-1}\alpha_{i,j}e_{i,j}\| + \|\sum_{i<j-1}\alpha_{i,j}e_{i+1,j}/2\| + \\ &+ \|\sum_{i<j-1}\alpha_{i,j}e_{i,j-1}/2\| + \|\sum_{i<j}\alpha_{i,j}e_{i-1,j}/2\| + \|\sum_{i<j}\alpha_{i,j}e_{i,j+1})/2\| \le \\ \le& \|2a\| + \|a/2\| + \|a/2\| + \|a/2\| + \|a/2\| = 4\|a\|.\end{aligned}$$

Therefore, $H'_\omega|_{S^1}$ is bounded.

□

PROPOSITION 5.3.3. *H''_ω is gapless.*

PROOF. By using the spectral theorem, stated in Theorem 5.2.13, it can be proven that if we have a unitary vector $|\varphi\rangle \in \bar{S}^1$ with $\langle\varphi|H'_\omega|\varphi\rangle = a$ which is orthogonal to the ground space of H'_ω, then $(0,a] \cap \sigma(H'_\omega) \neq \varnothing$.

Let us suppose that $\sigma(H'_\omega) \subseteq \{0\} \cup (a,\infty)$ to get a contradiction. In such a case, for E the spectral measure associated to H'_ω, the norm of $|\varphi\rangle$ would be

$$\langle\varphi|\varphi\rangle = \langle\varphi|E(\sigma(H'_\omega))|\varphi\rangle\langle\varphi| \int_{(a,\infty)} dE(z)|\varphi\rangle = 1$$

because $|\varphi\rangle$ is orthogonal to the ground space, and we would have that

$$a = \langle\varphi|H'_\omega|\varphi\rangle = \langle\varphi| \int_{\mathbb{R}^+} zdE(z)|\varphi\rangle \overset{|\varphi\rangle\in\ker(H'_\omega)^\perp}{=}$$

$$= \langle\varphi|\left(\int_{(0,a]} zdE(z) + \int_{(a,\infty)} zdE(z)\right)|\varphi\rangle \overset{\sigma(H'_\omega)\cap(0,a]=\varnothing}{=} \langle\varphi| \int_{(a,\infty)} zdE(z)|\varphi\rangle >$$

$$> \langle\varphi| \int_{(a,\infty)} adE(z)|\varphi\rangle = a\langle\varphi|\varphi\rangle = a.$$

Hence if such $|\varphi\rangle$ exists there must be some part of the spectrum lying in $(0,a]$.

The family of states

$$|\varphi_N\rangle = \sum_{\substack{-N<i<-1\\1<j<N}} |\cdots 00\rangle \otimes |0^{-N}0\cdots 0^i 11\cdots 1^j 0\cdots 0^N\rangle \otimes |00\cdots\rangle \in S_{-N,N},$$

which lie in S^1 and come from those states in eq. (29) embedded in our space, can be used together with the statement above to show that there exists a family $\{\lambda_n\}_{n=1}^\infty$ of elements in the spectrum of H''_ω which tends to 0. □

We will also use the fact that the residual spectrum of a self-adjoint operator is always empty, and a simple characterizacion of values contained in the point spectrum (σ_p) and continuous spectrum (σ_c) of an operator.

LEMMA 5.3.4. A value λ lies in $\sigma_p(L) \cup \sigma_c(L)$ for a given operator L defined on a Hilbert space $\mathcal{H}$ iff there exists a sequence of states $\{|\varphi_{\lambda,k}\rangle\}_{k=1}^\infty$ in $\mathcal{H}$ such that

$$\|(L-\lambda I)|\varphi_{\lambda,k}\rangle\| \overset{k\to\infty}{\to} 0.$$

The sequences in the previous lemma are called Weyl sequences[16], and are specially useful to identify values in the continuous spectrum. In the case of the operator H''_ω, there can be found Weyl sequences with a particular property.

PROPOSITION 5.3.5. *A real value $\lambda \in \mathrm{spec}(H''_\omega)$ iff there exists a sequence of states $\{|\psi_{\lambda,k}\rangle\}_k$ in S^1 such that $\|(H'_\omega - \lambda I)|\psi_{\lambda,k}\rangle\| \to 0$.*

[16]For values in the point spectrum the sequence could be constant by taking any associated eigenvector

Proof. This follows directly from the fact that the residual spectrum of H''_ω is empty –since it is self-adjoint–, the lemma above, and the fact that H''_ω is continuous.

Let $\{|\varphi_{\lambda,k}\rangle\}_{k=1}^{\infty}$ be a Weyl sequence for $\lambda \in \sigma_p(H''_\omega) \cup \sigma_c(H''_\omega)$.

Since S^1 is dense in the domain of H''_ω, which is continuous, for every k we can find a vector $|\psi_{k,\lambda}\rangle$ such that $\||\psi_{k,\lambda}\rangle - |\varphi_{\lambda,k}\rangle\| < 1/k|\lambda|$ and $\|H''_\omega(|\psi_{k,\lambda}\rangle) - H''_\omega(|\varphi_{\lambda,k}\rangle)\| < 1/k$.

Then,

$$\begin{gathered}\|H''_\omega(|\psi_{k,\lambda}\rangle) - \lambda|\psi_{k,\lambda}\rangle\| \leq \\ \leq \|H''_\omega(|\psi_{k,\lambda}\rangle) - H''_\omega(|\varphi_{\lambda,k}\rangle)\| + \|H''_\omega(|\varphi_{k,\lambda}\rangle) - \lambda|\varphi_{k,\lambda}\rangle\| + \|\lambda|\varphi_{k,\lambda}\rangle - \lambda|\psi_{\lambda,k}\rangle\| < \\ < 1/k + \|H''_\omega(|\varphi_{k,\lambda}\rangle) - \lambda|\varphi_{k,\lambda}\rangle\| + 1/k \to 0\end{gathered}$$

Therefore, $\{|\psi_{\lambda,k}\rangle\}_{k=1}^{\infty}$ is a Weyl sequence for λ contained in S^1. □

This last property lets us prove an 'additive' property on the spectrum, which will lead to the final result stating that the spectrum of the uncle Hamiltonian is the positive real line $\mathbb{R}^+$.

Proposition 5.3.6. *If two values a, b lie in the spectrum of H''_ω, then $a+b$ also lies in the spectrum of H'_ω.*

Proof. For both a and b we can find some sequences of states $\{|\psi_{a,k}\rangle\}_{k=1}^{\infty}$ and $\{|\psi_{b,k}\rangle\}_{k=1}^{\infty}$ contained in S^1 verifying the previous proposition. We can assume, due to translationally invariance of H''_ω and H'_ω, that the first sequence lies in $\bigcup_{i<-3} S_{i,-3}$, and the second one is contained in $\bigcup_{j>3} S_{3,j}$. Consequently each $|\psi_{a,k}\rangle$ is of the form $|\phi_{a,k}\rangle \otimes |0^{-2}00\cdots\rangle$, and similarly $|\psi_{b,k}\rangle = |\cdots 000^2\rangle \otimes |\phi_{b,k}\rangle$.

And due to the structure of H'_ω the image of $\bigcup_{i<-3} S_{i,-3}$ is contained in $\bigcup_{i<-1} S_{i,-1}$, and $H'_\omega(\bigcup_{j>3} S_{3,j}) \subseteq \bigcup_{j>1} S_{1,j}$.

If we consider the states $|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle$, then:

$$\begin{gathered}H'_\omega(|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle) = \\ = H'_\omega(|\phi_{a,k}\rangle) \otimes |0^0 00\rangle \otimes |\phi_{b,k}\rangle + |\phi_{a,k}\rangle \otimes |000^0\rangle \otimes H'_\omega(|\phi_{b,k}\rangle).\end{gathered}$$

And

$$\begin{gathered}\|(H'_\omega - (a+b)\mathbb{I})|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle\| = \\ = \|H'_\omega(|\phi_{a,k}\rangle) \otimes |0^0 00\rangle \otimes |\phi_{b,k}\rangle + |\phi_{a,k}\rangle \otimes |000^0\rangle \otimes H'_\omega(|\phi_{b,k}\rangle) - \\ -(a+b)|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle\| \leq \\ \leq \|H'_\omega(|\phi_{a,k}\rangle) \otimes |0^0 00\rangle \otimes |\phi_{b,k}\rangle - a|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle\| + \\ + \||\phi_{a,k}\rangle \otimes |000^0\rangle \otimes H'_\omega(|\phi_{b,k}\rangle) - b|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle\|,\end{gathered}$$

which tends to 0.

Hence, the sequence of states $|\phi_{a,k}\rangle \otimes |000^0 00\rangle \otimes |\phi_{b,k}\rangle$ is a Weyl sequence for $a+b$, and $a+b$ lies in $\mathrm{spec}(H'_\omega)$, as stated in the proposition. For longer sums of spectral values one only needs to consider the corresponding Weyl sequences and 'concatenate' them all.

□

THEOREM 5.3.7. $\sigma(H'_\omega) = [0, \infty)$.

PROOF. Let us first note that the set of finite sums of any sequence of real numbers tending to 0 is dense in $\mathbb{R}^+$.

From the previous result, it can be proven inductively that any finite sum of elements in the spectrum is also in the spectrum.

Since there exists a sequence of elements in $\sigma(H''_\omega)$ tending to 0 – at least the previous sequence $\{\lambda_n\}_n$ from Proposition 5.3.3– and any finite sum of these elements lies in $\sigma(H'_\omega)$, which is closed, this last spectrum must be the whole positive real line $\mathbb{R}^+$. There can be no more elements in the spectrum because H'_ω is a positive operator.

□

5.3.5. Gapless uncle Hamiltonians for unique ground states. Can we obtain uncle Hamiltonians with similar properties in the case of MPS which are unique ground states? Lemma 5.1.13 tells us that this cannot happen as long as the MPS tensors are injective, which is always the case as long as such an MPS is in its standard form: In that case, the uncle Hamiltonian is equal to the parent Hamiltonian. However, as we will demonstrate in the following, interesting uncle Hamiltonians can be obtained by choosing a different MPS representation.

Consider a qubit chain $(\mathbb{C}^2)^{\otimes N}$, and a state $|M(A)\rangle = |0\ldots0\rangle$. Clearly, this is a unique ground state of a gapped local Hamiltonian – with local term $h = \mathbb{I} - |00\rangle\langle 00|$–, with standard MPS representation $A_0 = (1)$, $A_1 = (0)$. However, we can write the same state with bond dimension 2 just by allowing repeated blocks, leading to the representation

$$A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } A_1 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

We can now perturb A with a perturbation P as in eq. (26), with $a_i = d_i$ and $b_i = c_i$[17], $i = 0, 1$. A calculation similar to the one for the GHZ state shows that in the limit of a vanishing perturbation, the ground space on three sites is $S_3 = \mathrm{span}\{|000\rangle, |W\rangle\}$, where $|W\rangle = (|001\rangle + |010\rangle + |001\rangle)/\sqrt{3}$ (as long as $b_1 \neq 0$); the uncle Hamiltonian h' is the projector onto $S_3^\perp$,

$$h' = \mathbb{I} - \big[|000\rangle\langle 000| + |W\rangle\langle W|\big] . \tag{30}$$

For an open chain of length n, $H' = \sum h'$ has the two ground states

$$\begin{aligned} |0_n\rangle &= |00\cdots0\rangle \quad \text{and} \\ |\mathrm{W}_n\rangle &= |100\cdots0\rangle + |010\cdots0\rangle + \ldots + |000\cdots01\rangle \ . \end{aligned}$$

Different from the GHZ case, the extra state $|W_N\rangle$ does not disappear from the kernel when closing the boundaries, and in this case the uncle Hamiltonian on a chain with periodic boundaries has a two-dimensional ground space, $\mathrm{span}\{|0_N\rangle, |W_N\rangle\}$. Note, however, that the thermodynamic limit of $|0_N\rangle$ and $|W_N\rangle$ is the same[18], and thus, the ground space

[17] This condition is needed for this specific construction because in other case first order terms in the diagonal blocks, and second order terms in the off-diagonal blocks, would add additional ground states to the local Hamiltonian, due to the repeated blocks.

[18] In the limit, they yield the same statistics by measuring local observables.

collapses to the original one in the thermodynamic limit.

Again, we can construct gapless excitations by considering the states

$$|\phi_n\rangle = \sum_{i\neq j} |0\cdots01^i00\cdots01^j0\cdots0\rangle \ .$$

As before, they are orthogonal to the ground space, and their energy is $O(1/N)$. Alternatively, we could have also chosen W states with momentum[19],

$$|\varphi_{N,k}\rangle = \sum_j e^{\frac{2\pi ikj}{N}} |0\cdots001^j00\cdots0\rangle,\ k \neq 0 \ ,$$

which are also orthogonal to the ground space, and have energy $O(k^2/N^2)$.

The spectrum is again dense in $\mathbb{R}^+$ in the thermodynamic limit. This can once more be verified by a mapping to the XY model (as we will see in the next section) or, directly in the thermodynamic limit, using the methods described before and in Sec. 5.4.4.

5.3.6. Relation to the XY model. Both the uncle Hamiltonian for the GHZ state and for the $|0\dots0\rangle$ state are closely related to the XY model (or, equivalently, to non-interacting fermions), which can be used to immediately infer that they are gapless models with spectra equal to $\mathbb{R}^+$. Let us first consider the uncle Hamiltonian for the GHZ state, eq. (28): It can be rewritten as

$$h' = -\tfrac{1}{4}\big(\mathbb{I}\otimes Z\otimes Z + Z\otimes Z\otimes\mathbb{I} + \mathbb{I}\otimes X\otimes\mathbb{I} - Z\otimes X\otimes Z\big) + \tfrac{1}{2}\mathbb{I}\otimes\mathbb{I}\otimes\mathbb{I} \ . \tag{31}$$

This is exactly the Hamiltonian discussed in eq. (11) from [**135**] at $g = 0$[20]. It can be solved either by transforming it to non-interacting fermions, or by a duality transformation to the XY model [**103**] [21]. The resulting Hamiltonian is

$$H_{XY} = -\tfrac{1}{4}\sum_i \big(X_i\otimes X_{i+1} + Y_i\otimes Y_{i+1} + 2Z_i \big) + \text{const.}$$

Indeed, this point in the XY model, which can be solved exactly by mapping it to non-interacting fermions [**76**], is known to be gapless with spectrum $\mathbb{R}^+$.

Let us now turn to the uncle Hamiltonian (30) for the $|0\dots0\rangle$ state. Let us first replace the uncle Hamiltonian with a simpler one with the similar spectral gap properties. Namely, let

$$\tilde{h}' = \mathbb{I} - |00\rangle\langle00| - |\Phi^+\rangle\langle\Phi^+| \ , \tag{32}$$

with $|\Phi^+\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$. We have that

$$\tfrac{1}{2}h' \le \tfrac{1}{2}(\tilde{h}'_{12} + \tilde{h}'_{23}) \le h' \ ,$$

which implies that for any finite chain, the ordered eigenvalues λ_i of $H' = \sum h'$ and $\tilde{\lambda}_i$ of $\tilde{H}' = \sum \tilde{h}'$ are related by

$$\tfrac{1}{2}\lambda_i \le \tilde{\lambda}_i \le \lambda_i \ .$$

[19]A state $|\varphi\rangle$ in a chain of length n is said to have momentum k if $\tau(|\varphi\rangle) = e^{k\frac{2\pi i}{n}}|\varphi\rangle$, where τ is the translation operator from Definition 5.1.4

[20]In fact, the construction in eq. (10) of [**135**] is, up to a gauge transformation, equivalent to the uncle construction, with $\varepsilon = \sqrt{g}$.

[21]The partial isometry $T : |i_1,\dots,i_N\rangle \mapsto |i_1 + i_2,\dots,i_N + i_1\rangle$ from the eigenspace of $X^{\otimes N}$ associated to the value 1 to the even Z parity space induces the duality mapping $X_i \mapsto T\circ X_i\circ T^{-1} = X_{i-1}\otimes X_i$ and $Z_i\otimes Z_{i+1} \mapsto T\circ(Z_i\otimes Z_{i+1})\circ T^{-1} = Z_i$.

I.e., if we want to determine essential spectral properties of H', such as whether its spectrum is not discrete, we can equally well study $\tilde{H}'$. Since $\tilde{h}'$ can be rewritten as

$$\tilde{h}' = -\tfrac{1}{4}\big(X \otimes X + Y \otimes Y + Z \otimes \mathbb{I} + \mathbb{I} \otimes Z\big) + \tfrac{1}{2}\mathbb{I} \otimes \mathbb{I} \ ,$$

this yet again gives rise to the same point of the XY model, eq. (31), proving that the Hamiltonians from local interactions in eqs. (30) and (32) have $\mathbb{R}^+$ as spectrum.

5.4. Properties of the uncle Hamiltonians for non-injective MPSs.

In this section, we will see that the observations we made for the uncle Hamiltonian for the GHZ state generalize to uncle Hamiltonians for arbitrary MPS with degenerate ground states (under some generic conditions): Their ground state space is equal to the ground state space of the parent Hamiltonian, they are gapless, and their spectrum is the whole positive real line. This section will also contain some proofs which have been omitted for the special case of the GHZ state.

For simplicity, we will focus here on the case where the MPS tensor C_i in its standard form, Theorem 5.1.7, has only two blocks, $C_i = A_i \oplus B_i$, but the same procedure can be followed in the general case: The results are completely analogous in case of multiple different blocks, but there are some differences if there are blocks with a multiplicity larger than one. We will comment on this particular case in Section 5.5.

Thus, in this section we will be dealing with an MPS $|M(C)\rangle$, for

$$C = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} ,$$

where both A and B are injective. We will choose A and B in the normal form of Theorem 5.1.7. The parent Hamiltonian for this MPS consists of local projectors $\Pi[C \overset{c}{-} C]$ with kernels

$$\operatorname{span}\{C \overset{c}{-} C\} = \operatorname{span}\{A \overset{c}{-} A\} + \operatorname{span}\{B \overset{c}{-} B\} \ ,$$

and the two-dimensional ground state space is spanned by $|M(A)\rangle$ and $|M(B)\rangle$.

5.4.1. Form of the uncle Hamiltonian. We will now determine the general form of the uncle Hamiltonian.

THEOREM 5.4.1. *Let $|M(C)\rangle$, be an MPS with block-injective $C = A \oplus B$, and let*

$$P = \begin{pmatrix} P^A & R \\ L & P^B \end{pmatrix}$$

be an arbitrary tensor, such that the 'uncle tensor'

$$U = \begin{pmatrix} A \overset{c}{-} A & A \overset{c}{-} R + R \overset{c}{-} B \\ B \overset{c}{-} L + L \overset{c}{-} A & B \overset{c}{-} B \end{pmatrix} . \tag{33}$$

is injective. Then, the uncle Hamiltonian induced by P exists and is a sum of local terms $h'_P = \Pi[U]$.

PROOF. Consider a perturbation $C_\varepsilon = C + \varepsilon P$ of the MPS $|M(C)\rangle$. We have that

$$C_\varepsilon \overset{c}{-} C_\varepsilon = \begin{pmatrix} A \overset{c}{-} A + O(\varepsilon) & \varepsilon(A \overset{c}{-} R + R \overset{c}{-} B) + O(\varepsilon^2) \\ \varepsilon(B \overset{c}{-} L + L \overset{c}{-} A) + O(\varepsilon^2) & B \overset{c}{-} B + O(\varepsilon) \end{pmatrix} .$$

Clearly, for $\varepsilon \neq 0$ the map $\mathcal{L}_\varepsilon$ which multiplies the off-diagonal blocks by $1/\varepsilon$ is invertible and thus (following Lemma 5.1.12)

$$\Pi[C_\varepsilon \overset{C}{-} C_\varepsilon] = \Pi[\mathcal{L}_\varepsilon(C_\varepsilon \overset{C}{-} C_\varepsilon)] = \Pi[U + O(\varepsilon)]\ .$$

Following Lemma 5.1.13, the limit $\lim_{\varepsilon\to 0} \Pi[U + O(\varepsilon)]$ exists whenever U is injective, and equals $\Pi[U]$. ☐

The required injectivity of the tensor in eq. (33) follows in particular from the following condition on the perturbation.

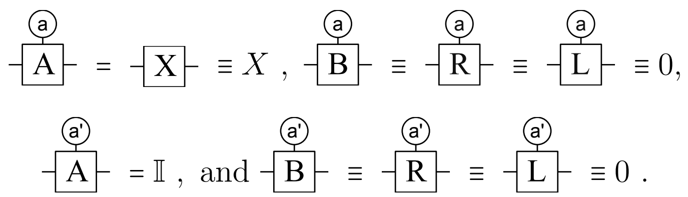
DEFINITION 5.4.2 (Injective perturbation). A perturbation P of an MPS $|M(C)\rangle$ (in the notation of Theorem 5.4.1) is called injective if

$$\begin{pmatrix} A & R \\ L & B \end{pmatrix} \tag{34}$$

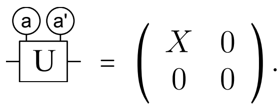
is an injective tensor.

LEMMA 5.4.3. *If a perturbation P is injective, then the resulting uncle tensor U, eq. (33), is injective.*

PROOF. Let us consider condition 5 from Lemma 5.1.10, and any X of the dimensions of $A\overset{c}{-}A$. Since the perturbation tensor is injective, there exist vectors $|a\rangle$ and $|a'\rangle$ such that



The product $|a\rangle \otimes |a'\rangle$ yields then for the uncle tensor



A similar reasoning can be followed for the rest of blocks, thus satisfying condition 5 from Lemma 5.1.10. ☐

A perturbation P is generically injective if $d \geq D^2$, and we will assume injective perturbations in the following. Note that unlike for the $|\mathrm{GHZ}\rangle$ state, the uncle Hamiltonian does in general depend on the perturbation (though only on its off-diagonal blocks R and L).[22]

[22] If $D \leq d < D^2$ and U [eq. (33)] is injective one can construct both parent and uncle Hamiltonians from projectors onto the span of three consecutive sites – this is what we did for the GHZ example. Then, the uncle Hamiltonian is the projector associated to

$$\begin{pmatrix} A\overset{c}{-}A\overset{c}{-}A & A\overset{c}{-}A\overset{c}{-}R + A\overset{c}{-}R\overset{c}{-}B + R\overset{c}{-}B\overset{c}{-}B \\ B\overset{c}{-}B\overset{c}{-}L + B\overset{c}{-}L\overset{c}{-}A + L\overset{c}{-}A\overset{c}{-}A & B\overset{c}{-}B\overset{c}{-}B \end{pmatrix}.$$

While we will restrict to injective perturbations for clarity, the same steps can be followed assuming only injectivity of U.

5.4.2. Ground space of the uncle Hamiltonian. In the following, we study the ground state space of the uncle Hamiltonian. Throughout, we will restrict to injective perturbations.

Let us first state the main result of this section, whose proof will be divided into two lemmas.

THEOREM 5.4.4. *Let P be an injective perturbation of an MPS $|M(C)\rangle$, $C = A \oplus B$. Then, the ground space of the uncle Hamiltonian H'_P is spanned by $|M(A)\rangle$ and $|M(B)\rangle$, and thus equal to the ground space of the parent Hamiltonian.*

The parent Hamiltonian is frustration free, i.e., its ground states minimize the energy of each local term. The ground space is thus

$$\ker(H) = \bigcap \ker(h) \ .$$

Since $\ker(h) \subset \ker(h'_P)$, it follows that

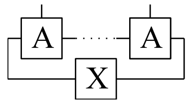
$$\ker(H'_P) = \bigcap \ker(h'_P) \supset \ker(H) \ ,$$

i.e., the uncle Hamiltonian is also frustration free, and any ground state of the parent is also a ground state of the uncle.

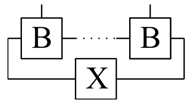
In order to classify all states in $\ker(H'_P) = \bigcap \ker(h'_P)$, we will follow the same steps as for the proof of the ground space structure of the parent Hamiltonian [**114**]: First, we will prove inductively how the ground space on a chain with open boundaries, $\bigcap_{i=1}^{k} \ker h'_{P,i,i+1}$, grows – the *intersection property*. Then, we will show how the ground space changes when we close the boundaries – the *closure property*.

LEMMA 5.4.5 (Intersection property). *Given a chain of length n, let S_n be the vector space*

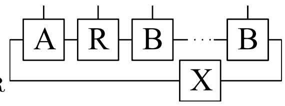
(35) $$S_n = A_n + B_n + R_n + L_n \ , \ \text{where}$$

$A_n = \Big\{$ 

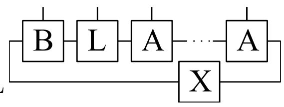
$/X \in \mathcal{M}_l\Big\}$,

$B_n = \Big\{$ 

$/X \in \mathcal{M}_m\Big\}$,

$R_n = \Big\{ \sum_{\text{pos R}}$ 

$/X \in \mathcal{M}_{l\times m}\Big\}$,

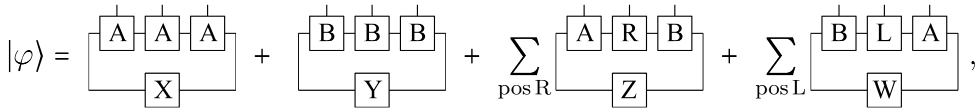
$L_n = \Big\{ \sum_{\text{pos L}}$ 

$/X \in \mathcal{M}_{m\times l}\Big\}$,

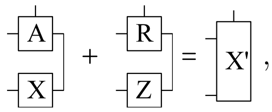
where the sums run over all possible positions of the R or L, padded with A's and B' to the left and right as indicated. Further, let $\left(\begin{smallmatrix} A & R \\ L & B \end{smallmatrix}\right)$ be injective. Then, the intersection property $S_n \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_n = S_{n+1}$ holds.

PROOF. We start by proving $S_2 \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_2 = S_3$. The proof will straightforwardly generalize to $S_k \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_k = S_{k+1}$, $k > 2$.

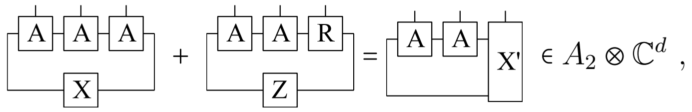
Let us first show that $S_2 \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_2 \supseteq S_3$. To this end, let $|\varphi\rangle \in S_3$, i.e., there exist X, Y, Z, and W such that

(36) 

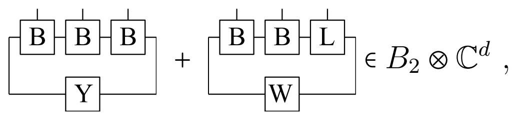
where the sums run over the three possible positions of R and L, respectively. If we now define

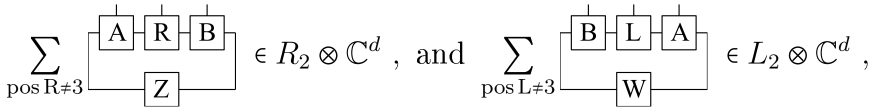
(37) 

we have that



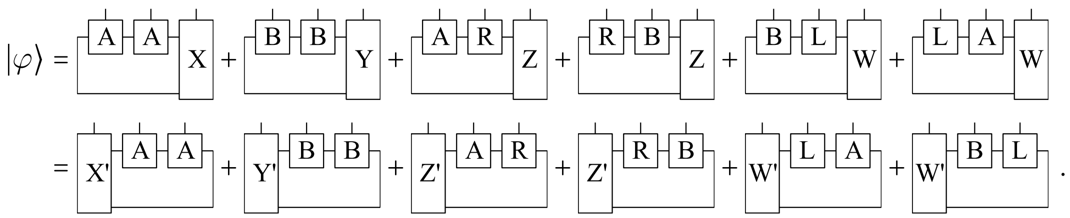
and similarly

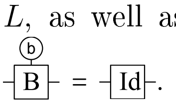


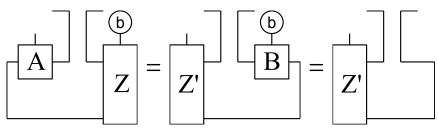


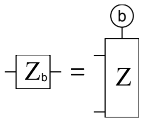
showing that $|\varphi\rangle \in S_2 \otimes \mathbb{C}^d$. Similarly, one can show that $|\varphi\rangle \in \mathbb{C}^d \otimes S_2$, proving that $S_2 \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_2 \supset S_3$.

Let us now show that conversely, $S_2 \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_2 \subseteq S_3$. Let $|\varphi\rangle \in S_2 \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_2$, i.e., there exist tensors X, Y, etc., such that

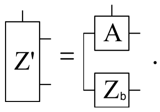
(38) 

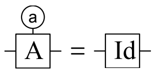
We want to show that $|\varphi\rangle$ is of the form (36), i.e., we need to show that X has a decomposition such as in (37), and so on. To this end, we will make heavy use of Lemma 5.1.10. In particular, injectivity of $\left(\begin{smallmatrix} A & R \\ L & B \end{smallmatrix}\right)$ implies the existence of a tensor R^{-1} left-inverse to R, which at the same time annihilates any of the other tensors A, B, and L, as well as the existence of a vector $|b\rangle$ satisfying condition 5 in Lemma 5.1.10 for . We now apply R^{-1} to the second site in eq. (38), which cancels all terms except one at each side of (38). Additionally, we project the third site onto $|b\rangle$ and obtain

(39) 

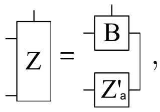
By defining  , we obtain that

(40)



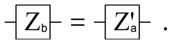
Similarly, we can apply A^{-1} at the second site and a vector $|a\rangle$ verifying condition 5 in Lemma 5.1.10 such that  at the first site to see that

(41)



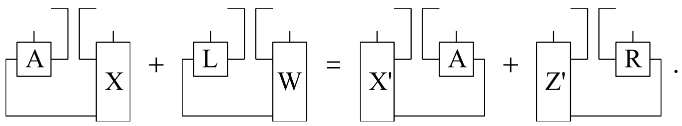
where Z'_a is defined correspondingly. Finally, we can project eq. (41) onto $|b\rangle$ to infer that

(42)

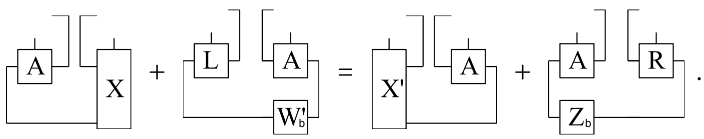


Corresponding expressions for the form of W and W' can be derived using L^{-1}.

Now let us return to the identity (38) and apply A^{-1} to the second site, which yields

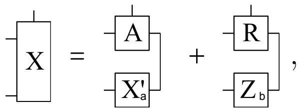


Using the analogue of eqs. (40–42) for W, this is equivalent to



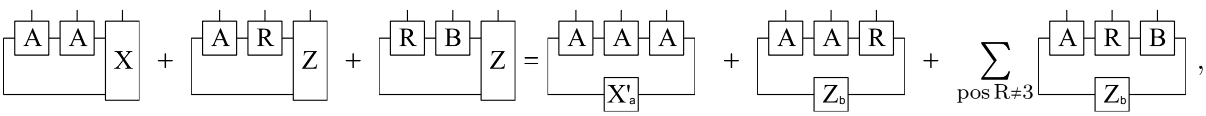
Now, we apply $|a\rangle$ to the first site and obtain

(43)



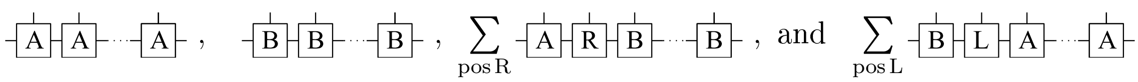
where we have defined X'_a accordingly.

Combining eqs. (41), (42), and (43), we find that



which shows that the left hand side, which is half of the terms in eq. (36), is contained in $A_3 + R_3$. In the same way it can be shown that the sum of other three terms in eq. (36) is contained in $B_3 + L_3$, which proves that $S_2 \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_2 \subset S_3$.

The proof that $S_k \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes S_k \subset S_{k+1}$ can be carried out in the same fashion, using that each of the tensors



have inverses which anihilate the rest of the tensors, since injectivity of $\left(\begin{smallmatrix} A & R \\ L & B \end{smallmatrix}\right)$ implies injectivity of

$$\begin{pmatrix} A \overset{c}{-} A \overset{c}{-} \cdots \overset{c}{-} A & \sum_{\text{pos R}} A \overset{c}{-} R \overset{c}{-} B \overset{c}{-} \cdots \overset{c}{-} B \\ \sum_{\text{pos L}} B \overset{c}{-} L \overset{c}{-} A \overset{c}{-} \cdots \overset{c}{-} A & B \overset{c}{-} B \overset{c}{-} \cdots \overset{c}{-} B \end{pmatrix} ;$$

this can be proven in analogy to Lemma 5.4.3. □

Starting from $S_2 = \ker(h'_{1,2})$, and using that

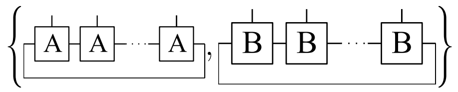
$$\bigcap_{i=1}^{k} \ker(h'_{i,i+1}) = \bigcap_{i=1}^{k-1} \ker(h'_{i,i+1}) \cap \bigcap_{i=2}^{k} \ker(h'_{i,i+1}) \ ,$$

the lemma allows to inductively prove that the ground space on n consecutive sites with open boundaries is $\bigcap_{i=1}^{n-1} \ker(h'_{i,i+1}) = S_n$: It differs from the ground space of the parent Hamiltonian by the presence of the 'zero momentum domain wall states' R_n and L_n, analogous to the domain wall states for the GHZ uncle. It remains to show that these states disappear from the kernel when closing the boundaries.

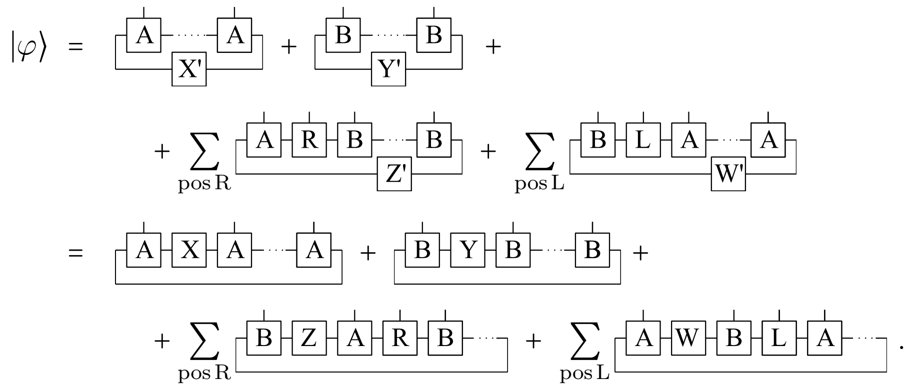
LEMMA 5.4.6 (Closure property). *Consider a chain of length N, and let $S_{\text{left}} = S_N$ defined on sites $1, \ldots, N$, and $S_{\text{right}} = S_N$ defined on sites $2, \ldots, N, 1$, using the definitions of the previous lemma. (I.e., for S_{right} the ordering of sites is shifted cyclically by one.) Then,*

$$S_{\text{left}} \cap S_{\text{right}} = \mathrm{span}\left\{|M(A)\rangle, |M(B)\rangle\right\} .$$

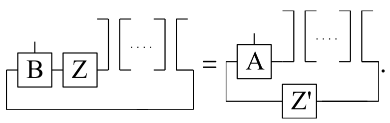
PROOF. It is clear that

$S_{\text{left}} \cap S_{\text{right}} \supset \mathrm{span}$ 

To show the converse, let $|\varphi\rangle \in S_{\text{left}} \cap S_{\text{right}}$:



By applying the inverse tensor corresponding to $\sum_{\text{pos R}} \boxed{A}\boxed{R}\boxed{B}\cdots\boxed{B}$ at sites $2, \ldots, N$, we get



Now let $|a\rangle$ be such that $\overset{a}{\boxed{A}} = \boxed{\mathrm{Id}}$ and $\overset{a}{\boxed{B}} = 0$ (Lemma 5.1.10): Projecting the first site onto $|a\rangle$ yields $\boxed{Z'} = 0$; with a corresponding $|b\rangle$, we find that $\boxed{Z} = 0$. In the same way, we can prove that $\boxed{W'} = \boxed{W} = 0$.

Now, we can apply A^{-1} to all sites to find that $-\boxed{\mathrm{X}}- = -\boxed{\mathrm{X'}}- = -\boxed{\mathrm{Id}}-$, and B^{-1} to obtain $-\boxed{\mathrm{Y}}- = -\boxed{\mathrm{Y'}}- = -\boxed{\mathrm{Id}}-$ (a similar proof can be found in [**114**]), showing that

$$S_{\text{left}} \cap S_{\text{right}} \subset \operatorname{span}\{|M(A)\rangle, |M(B)\rangle\}\,.$$

□

The closure property shows that if we close the boundaries on a chain of length N, we indeed recover the ground space of the parent Hamiltonian, since

$$\bigcap_{i=1}^{N} \ker(h'_{i,i+1}) = \bigcap_{i=1}^{N-1} \ker(h'_{i,i+1}) \cap \bigcap_{i=2}^{N} \ker(h'_{i,i+1}) = S_{\text{left}} \cap S_{\text{right}}\ .$$

Together, the two lemmas thus prove Theorem 5.4.4.

5.4.3. Gaplessness of the uncle Hamiltonian on finite chains. One of the key properties of the parent Hamiltonian is that it exhibits a spectral gap above the ground space [**41, 86**]. On the other hand, as we will prove in the following the uncle Hamiltonian is generically gapless:

Theorem 5.4.7. *The uncle Hamiltonian H'_P is gapless for almost every P.*

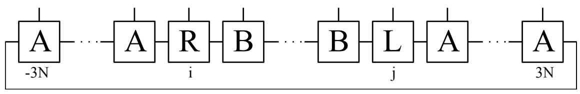
The Theorem can be proven using the following Lemma:

Lemma 5.4.8. *For a chain of length $6N+1$, let*

$$|\phi_N\rangle = \sum_{\substack{-2N\le i\le -N\\ N\le j\le 2N}} |\zeta_{i,j}\rangle\ , \tag{44}$$

where

$|\zeta_{i,j}\rangle$ =



.

Then, for almost every R and L (and thus almost every P), the following holds:

(1) $\langle\phi_N|\phi_N\rangle = \Theta(N^2)$.
(2) $\langle M(A)|\phi_N\rangle = O(e^{-N})$ *and* $\langle M(B)|\phi_N\rangle = O(e^{-N})$.
(3) $\langle\phi_N|H'_P|\phi_N\rangle = O(N)$.

Here, $\Theta(\cdot)$ denotes both lower and upper bounds on the scaling.

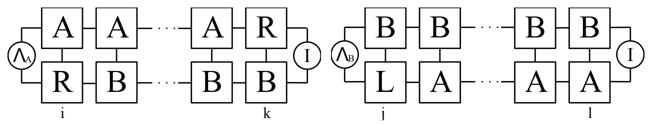
Note that $|\phi_N\rangle$ generalizes the GHZ 'boundary wall' ansatz for low energy states, eq. (29). The range for i and j in (44) is chosen such that R and L move over a region of size N each, leaving two separating regions of length $2N$ each which contain only A or B tensors, respectively.

Proof of Theorem 5.4.7. For the normalized states $|\hat{\phi}_N\rangle := |\phi_N\rangle/\||\phi_N\rangle\|$ on a chain of length $6N+1$ (with $|\phi_N\rangle$ from Lemma 5.4.8), we have that $|\hat{\phi}_N\rangle$ tends to be orthogonal to the ground space of H'_P and $\langle\hat{\phi}_N|H'_P|\hat{\phi}_N\rangle \to 0$ as $N\to\infty$. Together with simple spectral decomposition arguments[23], this implies the existence of a sequence $\delta_N \to 0$ such that H'_P (on $6N+1$ sites[24]) has at least one eigenvalue in the interval $(0,\delta_N)$. □

[23]This can be proven with a finite-dimensional version of the proof of Theorem 5.4.10.
[24]The producedure can be easily tuned for long chains not of this type.

PROOF OF LEMMA 5.4.8. (1) $\langle\phi_N|\phi_N\rangle = \Theta(N^2)$*:* Lemma 5.1.8 allows us to approximate

$$\langle\zeta_{i,j}|\zeta_{k,l}\rangle =$$



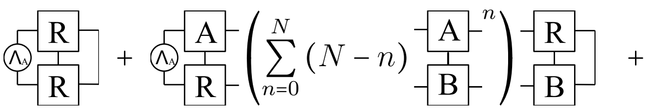
$$+\,O(e^{-2N})\ ,$$

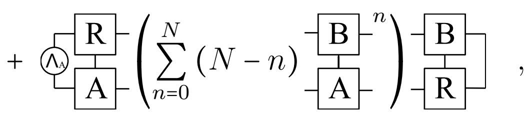
for $i<k$ and $j<l$, and correspondingly for the other cases.

Note that we have used $\rho(E^A_B) = \rho(E^B_A) \le 1$, Lemma 5.1.9, together with eq. (20) to bound the error term.

Now it follows that $\langle\phi_N|\phi_N\rangle = \Xi_R\Xi_L + O(e^{-2N})$, with

$$\Xi_R := (N+1)$$

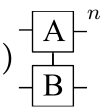




and correspondingly for Ξ_L.

Since the spectral radius of E^A_B is lower that 1, we have that the middle part of the previous second summand is

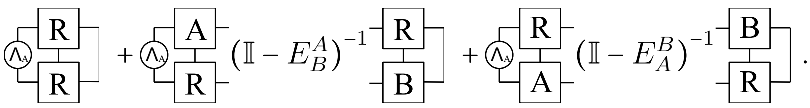
$$\sum_{n=0}^{N}(N-n)$$



$$= \frac{N\mathbb{I} - \frac{E^A_B-(E^A_B)^{N+1}}{\mathbb{I}-E^A_B}}{\mathbb{I}-E^A_B} = \frac{N\mathbb{I}}{\mathbb{I}-E^A_B} - \frac{E^A_B-(E^A_B)^{N+1}}{(\mathbb{I}-E^A_B)^2}\ ,$$

where the second summand in this last equation has as limit $-\frac{E^A_B}{(\mathbb{I}-E^A_B)^2}$. An analogue procedure can be followed for the part involving E^B_A to finally find that $\Xi_R = C_R N + O(1)$, with

$$C_R =$$

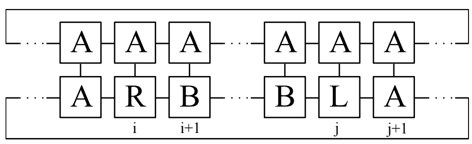


C_R is a quadratic function in R which does not vanish identically (e.g., there exists an R for which $\Pi_R\Pi_A = 0$ and the first term is non-zero). Thus, the R for which $C_R = 0$ form an algebraic variety of smaller dimension, and $C_R \neq 0$ for almost all R.[25]

The same argument can be used to see that $\Xi_L = C_L N + O(1)$ where $C_L \neq 0$ for almost all L, and thus, $\langle\phi_N|\phi_N\rangle = \Theta(N^2)$ for almost every perturbation as claimed.

(2) $\langle M(A)|\phi_N\rangle = O(e^{-N})$ *and* $\langle M(B)|\phi_N\rangle = O(e^{-N})$*:* In the scalar product

$$\langle M(A)|\phi_N\rangle = \sum_{\substack{-2N\le i\le -N\\ N\le j\le 2N}}$$



,

[25]If $\Pi_A\Pi_B = 0$, i.e., $E^A_B = 0$, such as for the GHZ state, one can prove that $C_R \neq 0$ for any injective perturbation.

every summand contains $(E_B^A)^{2N}$. Using Lemma 5.1.9 and the fact that there are only $O(N^2)$ summands, $\langle M(A)|\phi_N\rangle = O(e^{-N})$ follows, and analogously for $\langle M(B)|\phi_N\rangle$.

(3) $\langle\phi_N|H_P'|\phi_N\rangle = O(N)$*:* The only terms in H_P' which give a non-zero energy are $h'_{-2N-1,-2N}$, $h'_{-N,-N+1}$, $h'_{N-1,N}$, and $h'_{2N,2N+1}$. For each of them, $N+1$ summands in (44) contribute, and thus, $\langle\phi_N|H_P'|\phi_N\rangle = O(N)$. □

5.4.4. Spectrum of the uncle Hamiltonian. In order to study more properties of the spectra of the uncle Hamiltonians we need to move on to the thermodynamic limit, introduced in Section 5.2.3.

The algebra we are dealing with is the completion of the algebra of local observables over an infinite spin chain:

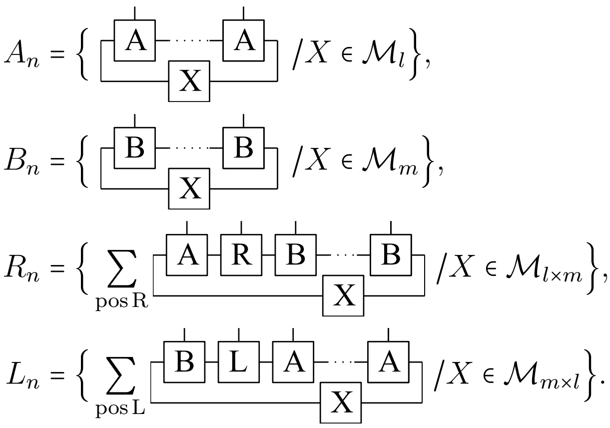
$$\mathcal{A} = \bigcup_{i<j} \cdots \otimes \mathbb{I} \otimes \mathbb{I} \otimes \mathcal{A}_i \otimes \mathcal{A}_{i+1} \otimes \cdots \otimes \mathcal{A}_j \otimes \mathbb{I} \otimes \cdots, \tag{45}$$

where each $\mathcal{A}_k$ denotes the local algebra of observables at the respective site k. Since the dimension at each site is always the same in translationally invariant MPSs, this local algebra is the same for every site, say $\mathcal{B}$.

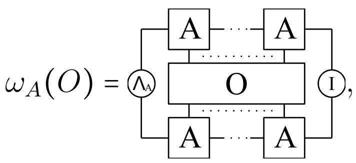
Even though the limit we must take is that of the evolutions determined by the finitely supported Hamiltonians in this algebra, let us give some intuitive description of the 'limit states' which will help us understand the ideas behind and will let us take an MPS-like description for the thermodynamic limit.

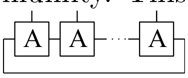
Recall from Section 5.4.2 that, for open boundary conditions, the ground state space for a finite lattice is the vector space

$$S_n = A_n + B_n + R_n + L_n \ , \text{ where} \tag{46}$$

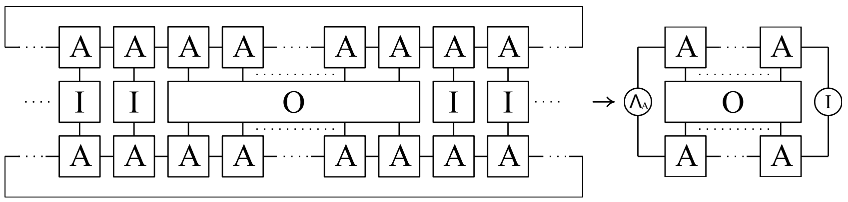


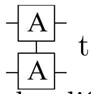
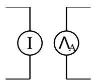
However, the thermodynamic limit of all these states lie in a 2-dimensional vector space. Let ω_A be the state densely defined on local observables O as

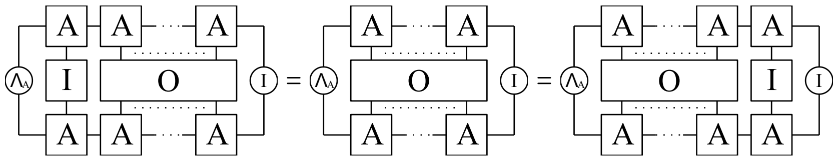


and extended by continuinity. This state can be considered as the limit of the unnormalized states $|M(A)\rangle =$ 

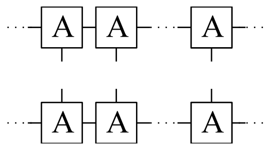
, since for any local observable O we have $\omega_A(O)$ as the limit



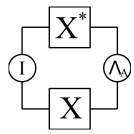
because the many copies of the operator  tend to  and $\mathrm{tr}(\Lambda_A) = 1$. Note that the definition of ω_A does not depend on the different regions an observable O might be considered to act at, since



Therefore, it is natural to describe ω_A as

$\omega_A =$  .

And, due to the injectivity of A, no matter which tensor X is chosen for the states in $\mathcal{A}_n$. For any X, and up to a normalization of the limit vectors by a constant



the limit is ω_A for every vector family in $\mathcal{A}_n$ for increasing n.

In a similar vein we can consider an analogue state ω_B as limit for the states in $\mathcal{B}_n$.

Let us note that ω_A and ω_B are normalized – i.e. they are in fact states on the algebra of local observables, and not only positive $*$-functionals – due to condition (3) of the standard form for MPSs (Theorem 5.1.7), since the value of $\omega_A(\mathbb{I})$ is exactly $\mathrm{tr}(\Lambda_A)$ (respectively $\mathrm{tr}(\Lambda_B)$), which was taken to be 1 when we defined the way to choose the matrices for an injective MPS.

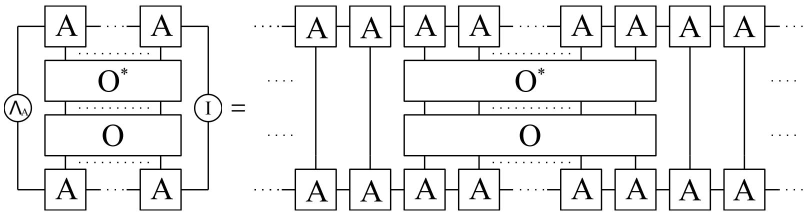
Informally, for a fixed observable, the limit of the states in $\mathcal{R}_n$ and $\mathcal{L}_n$ is $(\omega_A + \omega_B)/2$ if the growth of the chain is made at the same speed at both ends. This is due to the fact that the role of the tensors R and L becomes negligible when they lie far away from the location of the local observable, and the number of terms in which their contribution is significant is also negligible compared with the number of terms in which it is not. In the case another ratio of growth is considered, the limit will still be a convex linear combination of these two states. Therefore, uncle and parent Hamiltonians also share the ground state space in the thermodynamic limit for open boundary conditions.

For the GNS-representation, we can take $\omega = \omega_A$ as the state to which the representation is associated[26]. ω_A is certainly a ground state in the thermodynamic limit, for if we consider the uncle Hamiltonian with open boundary conditions at any finite sublattice $\Lambda \subset \mathbb{Z}$ – let us call it H'_Λ– we have

$$\begin{aligned}
-i\omega_A(O^*\delta(O)) &= -i\lim_{\Lambda\to\mathbb{Z}} \omega_A(O^*\delta_\Lambda(O^*)) = \lim_{\Lambda\to\mathbb{Z}} \omega_A(O^*H'_\Lambda O - O^*OH'_\Lambda) \\
&= \lim_{\Lambda\to\mathbb{Z}} \omega_A(O^*H'_\Lambda O) - \lim_{\Lambda\to\mathbb{Z}} \omega_A(O^*OH'_\Lambda) \\
&= \lim_{\Lambda\to\mathbb{Z}} \omega_A(O^*H'_\Lambda O) - 0 \geq 0
\end{aligned}$$

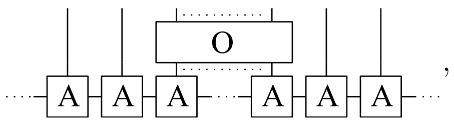
for every O in the domain of δ.

In the first place we have to construct the quotient of the C^*-algebra $\mathcal{U}_{\mathrm{loc}} = \overline{\mathcal{A}}$ of quasi-local observables by the ideal of those observables O such that $\omega_A(O^*O) = 0$:

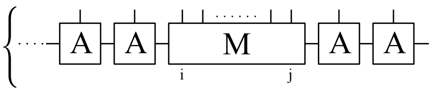


$= 0.$

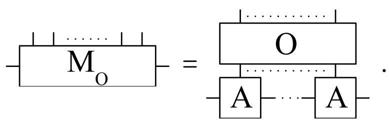
We can see this as the seminorm, induced by ω, of the vector



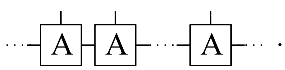
and the representatives ξ_O of the equivalence classes in the quotient will also have this form. Since any operator O can be considered, the Hilbert space of the representation will be seen as the completion of

$S = \bigcup_{i\leq j} S_{i,j}$, where $S_{i,j} = \mathrm{span}\Big\{$  $,\ M\Big\}$,

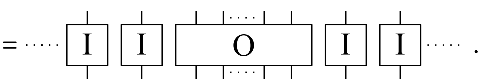
where the corresponding quotient should be taken into account (different tensors M can lead to the same states). Tensors M come from the contraction



Now we have the Hilbert space $\mathcal{H}_\omega = \bar{S}$, we just need the C^*-algebra representation $\pi_\omega : \overline{\mathcal{A}} \to B(\mathcal{H})$. As we took as distinguised vector Ω_ω of the cyclic representation the vector in $\bar{S}$ corresponding to the class determined by the identity, we first have

$\Omega_\omega = \xi_{\mathbb{I}} =$ 

For any local observable $\mathbb{I}\otimes O\otimes\mathbb{I}$ we have

$\pi_\omega(\mathbb{I}\otimes O\otimes\mathbb{I})(\Omega_\omega) = \xi_O \Rightarrow \pi_\omega(\mathbb{I}\otimes O\otimes\mathbb{I}) =$ 

[26]The choice of either ω_A or ω_B – or any convex linear combination of them – is irrelevant in this case, since they play a similar role in the parent Hamiltonian. However, for general Hamiltonians, the spectrum in the thermodynamic limit may depend on the ground space taken for the representation.

The global uncle Hamiltonian H'_P acting on $\mathcal{H}_\omega$, densely defined on S[27] as the infinite sum of the local terms $H'_P = \sum h'_{\text{loc}}$, coincides on S with the Hamiltonian H_ω arising from the representation, for it exactly implements the dynamics induced for every local observable.

Moreover, H'_P is essentially self-adjoint on $\mathcal{H}_\omega$.

PROPOSITION 5.4.9. The operator H'_P, densely defined on S, is essentially self-adjoint.

PROOF. H'_P is easily seen to be symmetric, because all its local summands h'_{loc} are orthogonal projections. Therefore, for H'_P to have a unique self-adjoint extension, it suffices to have a dense set of analytic elements in its domain.

If $|\varphi\rangle$ belongs to S, it must be in some $S_{-M,M}$. Note that, for every N, we have that $\|H'_P|_{S_{-N,N}}\| \le 2N+2$ and $H'_P(S_{-N,N}) \subseteq S_{-N-1,N+1}$, and therefore

$$\|{H'_P}^n(|\varphi\rangle)\| \le \Pi_{k=1}^n (2M+2k)\||\varphi\rangle\|.$$

From this we have

$$\frac{r^n}{n!}\|{H'_P}^n(|\varphi\rangle)\| \le r^n \Pi_{k=1}^n \frac{2M+2k}{k} \le r^n \Pi_{k=1}^n (2M+2) = r^n(2M+2)^n,$$

which is summable for $r < 1/(2M+2)$.

Thus every vector in S is an analytic vector for H'_P, which is therefore essentially self-adjoint.

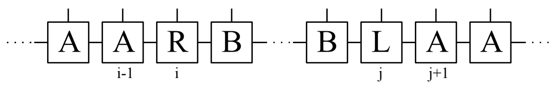
□

Consequently, the thermodynamic limit Hamiltonian H_ω is the unique self-adjoint extension of the global uncle Hamiltonian H'_P. Let us rename it as $H'_\omega = H_\omega$ so as to keep the reference to the uncle Hamiltonian it came from. Let us now study the spectral properties of this operator.

In the first place, we must show that H'_ω is gapless. A family of states related to those previously used for finite chains in Lemma 5.4.8 and Theorem 5.4.7 let us show the absence of gap:

$$|\phi_N\rangle = \sum_{\substack{-2N \le i \le -N \\ N \le j \le 2N}} |\zeta_{i,j}\rangle\ , \tag{47}$$

where

$|\zeta_{i,j}\rangle$ =  .

In addition to the spectral theorem, we will make use of the fact that H_ω is a self-adjoint operator. Therefore its residual spectrum is empty, and the whole spectrum is real [**32**]. Moreover, since it is a positive operator the spectrum is contained in $\mathbb{R}^+$.

THEOREM 5.4.10. *The uncle Hamiltonian H'_P is gapless in the thermodynamic limit for almost every P.*

[27]Note that since, given any element of S, only finitely many local Hamiltonians do not anihilate on it, this global uncle Hamiltonian is well defined on S.

Proof. We consider the operator H'_ω, which models the thermodynamic limit of H'_P with boundary conditions described by the A tensor, i.e. with chosen ground state $\omega = \omega_A$.

Recall that the bounds from Lemma 5.4.8 also apply to the states in (47).

With the Spectral Theorem in hand, it can be proven that if we have a unitary vector $|\varphi\rangle \in \bar{S}$ with $\langle\varphi|H'_\omega|\varphi\rangle = a$ which is orthogonal to the ground space of H'_ω, then $(0,a] \cap \sigma(H'_\omega) \neq \varnothing$. This can be done exactly in the same way it was done for the operator H''_ω when studying the uncle Hamiltonian for the GHZ state in Proposition 5.3.3.

Hence, if such $|\varphi\rangle$ exists there must be some part of the spectrum lying in $(0,a]$. However, for a general MPS, the low energy states we have found are not kwown to be orthogonal to the ground space. Therefore we cannot state that the projection $E(\{0\})$, associated to the spectral measure, plays no role when looking at these states, but we can say that it is negligible.

Since the states $|\phi_n\rangle$ tend to be orthogonal to the ground space, we have that the values of $\langle\phi_n|E(\{0\})|\phi_n\rangle$ tend to 0. We can consider $|\psi_n\rangle = |\phi_n\rangle - E(\{0\})|\phi_n\rangle$, with norm tending to 1 and orthogonal to Ω_ω.

The only difference from the proof in Proposition 5.3.3 is that from the fact that the energies of these states are close to a we cannot infer directly that an element from $(0,a]$ lies in the spectrum, but we can prove that some element from $(0,r]$ does for every $r > a$ and, therefore, also an element from $(0,a]$ does. If this were not the case, we would have that

$$
\begin{aligned}
a \sim \langle\psi_n|H'_\omega|\psi_n\rangle = \langle\psi_n| \int_{\mathbb{R}^+} z dE(z) |\psi_n\rangle &\overset{|\psi_n\rangle \in \ker(H'_\omega)^\perp}{=} \\
= \langle\psi_n| \left(\int_{(0,r]} z dE(z) + \int_{(r,\infty)} z dE(z) \right) |\psi_n\rangle &\overset{\sigma(H'_\omega)\cap(0,r]=\varnothing}{=} \\
= \langle\psi_n| \int_{(r,\infty)} z dE(z) |\psi_n\rangle &\geq \\
\geq \langle\psi_n| \int_{(r,\infty)} r dE(z) |\psi_n\rangle = r\langle\psi_n|\psi_n\rangle &\to r,
\end{aligned}
$$

which contradicts the hypothesis $r > a$. □

This last result shows the existence of a sequence of elements in $\sigma(H'_\omega)$ tending to 0

Proposition 5.4.11. *A real value $\lambda \in \operatorname{spec}(H'_\omega)$ iff there exists a sequence of normalized states $\{|\varphi_{\lambda,k}\rangle\}_k \in S$ such that $\|(H'_\omega - \lambda I)(|\varphi_{\lambda,k}\rangle)\| \to 0$.*

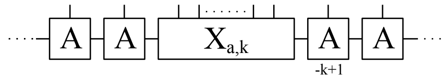
Proof. This follows from the fact that the residual spectrum of H'_ω is empty –since it is self-adjoint–, the characterization of a point lying in the point or continuous spectrum in Lemma 5.3.4, and the fact that H'_ω is the closure of H'_P acting on S, that is,

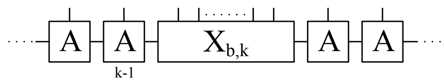
$$
\operatorname{graph}(H'_\omega) = \overline{\operatorname{graph}(H'_P|_S)} \subset \bar{S} \times \bar{S}.
$$

The proof is analogue to that provided in Proposition 5.3.5 □

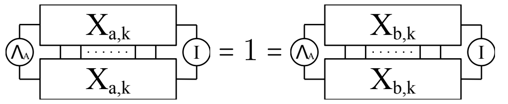
Proposition 5.4.12. *If some values a,b lie in the spectrum of H'_ω then the sum $a+b$ also lies in the spectrum of H'_ω.*

PROOF. For both a and b we can find some sequences of normalized states $\{|\varphi_{a,k}\rangle\}_{k=1}^{\infty}$ and $\{|\varphi_{b,k}\rangle\}_{k=1}^{\infty} \subset S$ verifying the previous proposition, with $\|H'_\omega(|\varphi_{c,k}\rangle) - |\varphi_{c,k}\rangle\| < 1/k$ for $c = a, b$. We can assume, due to translationally invariance of H'_ω, that the first sequence lies in $\bigcup_{i<-k} S_{i,-k}$, and the second one is contained in $\bigcup_{j>k} S_{k,j}$. These states would then have the form

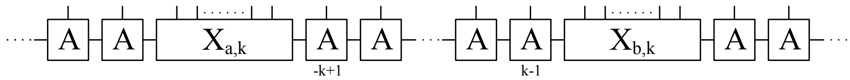
$|\varphi_{a,k}\rangle =$ 

$|\varphi_{b,k}\rangle =$  ,

for some tensors $X_{a,k}$, $X_{b,k}$. The normalization conditions on tensors A and B lead to

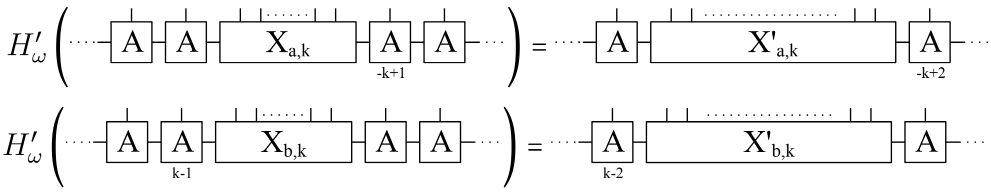


From these states we can consider the ‘concatenated’ states

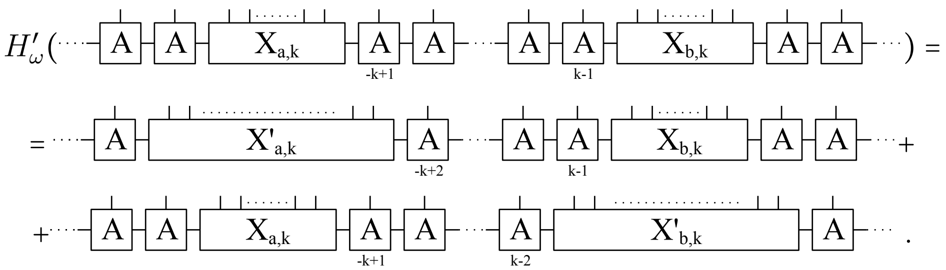
$|\Phi_k\rangle =$  ,

Note that the separation between the X blocks is increasingly growing.

Due to the structure of H'_ω, the image of $\bigcup_{i<-k} S_{i,-k}$ is contained in $\bigcup_{i<-k} S_{i,-k+1}$, and $H'_\omega(\bigcup_{j>k} S_{k,j}) \subseteq \bigcup_{j>k} S_{k-1,j}$. Moreover, there exist tensors $X'_{a,k}$ and $X'_{b,k}$ such that



These new tensors also allow us to describe the image of the concatenations:

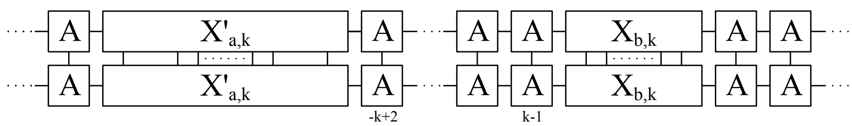


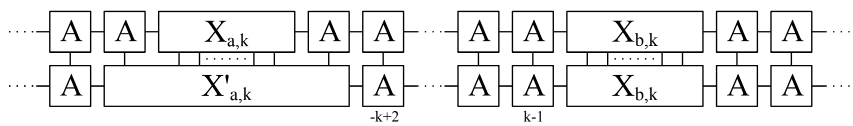
Let us call $|\Phi'_{k,a}\rangle$ and $|\Phi'_{k,b}\rangle$ these two summands respectively. We then have that

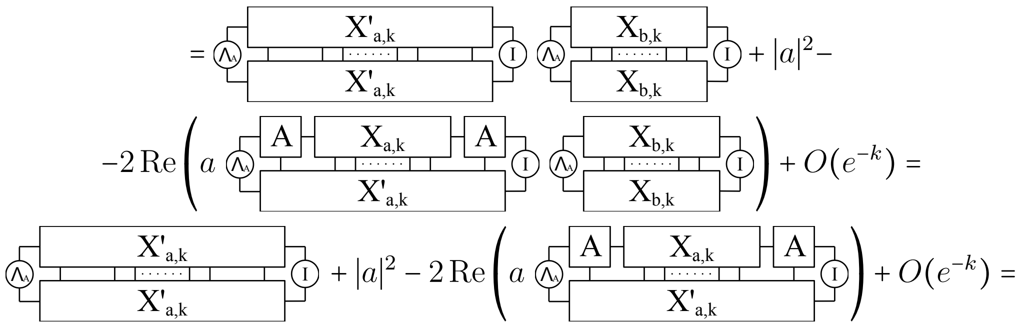
$$\|H'_\omega(|\Phi_k\rangle) - (a+b)|\Phi_k\rangle\| \leq \||\Phi'_{k,a}\rangle - a|\Phi_k\rangle\| + \||\Phi'_{k,b}\rangle - b|\Phi_k\rangle\|.$$

We can derive a bound for this first last summand:

$$\||\Phi'_{k,a}\rangle - a|\Phi_k\rangle\|^2 = \langle\Phi'_{k,a}|\Phi'_{k,a}\rangle + |a|^2\langle\Phi_k|\Phi_k\rangle - 2\,\mathrm{Re}(a\langle\Phi'_{k,a}|\Phi_k\rangle) =$$

 $+ |a|^2(1 + O(e^{-k}))-$

$-2\,\mathrm{Re}\Bigg(a$  $\Bigg) =$



$$= \|H'_\omega(|\varphi_{a,k}\rangle) - a|\varphi_{a,k}\rangle\|^2 + O(e^{-k}) < 1/k^2 + O(e^{-k}),$$

where $\mathrm{Re}(\cdot)$ denotes the real part.

A similar bound can be found for the second summand, and we can derive the bound

$$\|H'_\omega(|\Phi_k\rangle) - (a+b)|\Phi_k\rangle\| = O(1/k).$$

We also have that $\||\Phi_k\rangle\| \to 1$. Therefore, the sequence $|\Phi_k\rangle/\||\Phi_k\rangle\|$ satisfy the conditions in Proposition 5.4.11 for $a+b$, and consequently this sum lies in the spectrum of H'_ω.

□

Inductively, longer concatenations would prove the result for any finite sum among values from $\{\lambda_1, \ldots, \lambda_n\}$ known to be in the spectrum. Note that the bound we get depends on the number of values λ_i we are summing,

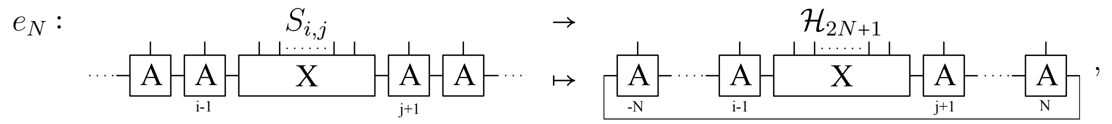
$$\left\| H'_\omega(|\Phi_k\rangle) - \left(\sum_{i=1}^{n} \lambda_i\right) |\Phi_k\rangle \right\| = O(n/k). \tag{48}$$

THEOREM 5.4.13. *The spectrum of the uncle Hamiltonian H'_P in the thermodynamic limit is the whole positive real line for almost every perturbation P.*

PROOF. Recall that the set of finite sums of any sequence of real numbers tending to 0 is dense in $\mathbb{R}^+$. Since there exists a sequence of elements in $\sigma(H'_\omega)$ tending to 0 – as it can be deduced from Theorem 5.4.10 – and any finite sum of these elements lies in $\sigma(H'_\omega)$, which is closed, this last spectrum must be equal to $\mathbb{R}^+$. Therefore the spectrum of H'_P is the whole positive real line. □

Spectra for finite chains. After this discussion on thermodynamic limit Hamiltonians we can go back to finite chains, and study how the spectra of the uncle Hamiltonians constructed on finite spin chains tend to be dense in $\mathbb{R}^+$ as the size of the chain grows.

Given $i < j$, $S_{i,j}$ can be easily mapped to any finite chain of lenght $2N+1 > j-i+1$ via



and this family of maps capture important information since they tend to be isometric embeddings.

LEMMA 5.4.14. *For fixed i and j, e_N is an isometry up to a correction $O(e^{-N})$.*

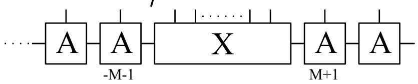
PROOF. It follows from Lemma 5.1.8. □

Since we will need to keep track of how close some vector evidencing the existence of elements in the spectrum is from being an eigenvector we introduce the following definition.

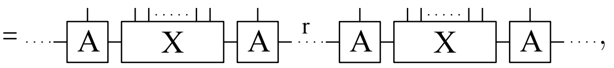
DEFINITION 5.4.15. A normal vector $|\varphi_{\lambda,k}\rangle$ will be called an approximated eigenvector for an operator A and a given value λ, and for an error ε if $\|(A-\lambda I)|\varphi_{\lambda,k}\rangle\| < \varepsilon$. In the case of a non-normalized vector it must satisfy

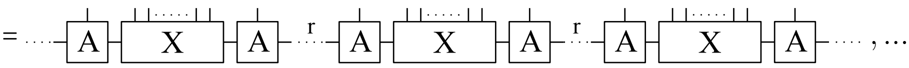
$$\frac{\|(A-\lambda I)(|\varphi_{\lambda,k}\rangle)\|}{\||\varphi_{\lambda,k}\rangle\|} < \varepsilon$$

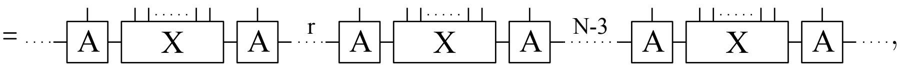
LEMMA 5.4.16. *For any given values $\lambda \in \mathbb{R}^+$, $n \in \mathbb{N}$ and $\delta > 0$, there exists a value N_0 such that we can find normalized approximated eigenvectors for the values $j\lambda$, $j = 1, \dots, n$, and for an error at most δ, for every finite chain with length greater that $2N_0 + 1$.*

PROOF. Let us take $\delta' = \delta/4n$. For λ and an error δ', a normalized approximated eigenvector $|\varphi_{\lambda,\delta}\rangle$ = 

can be found in some $S_{-M,M}$ such that $\|(H'_\omega - \lambda\mathbb{I})|\varphi_{\lambda,\delta}\rangle\| < \delta'$. We can now find a value r such that the following vectors are respectively approximated eigenvectors, not necessarily normalized, for the values $j\lambda$, $j = 2, \dots, n$, and an error[28] at most $2j\delta' < \delta/2$:

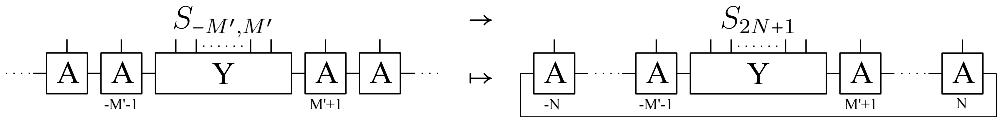
$|\varphi^{(2)}_{\lambda,\delta}\rangle$ = 

$|\varphi^{(3)}_{\lambda,\delta}\rangle$ = 

$|\varphi^{(N)}_{\lambda,\delta}\rangle$ = 

where the r denotes how many A tensors are missing in the diagram, and the $N-3$ refers to the number of X blocks, with r copies of tensor A between every two of them, which are also missing.

A value M' can be found such that all these states belong to $S_{-M',M'}$. And, due to Lemma 5.4.14, there exists a value N_0 such that the maps

e_N : 

make each $e(|\varphi^{(i)}_{\lambda,\delta}\rangle)$ an approximated eigenvector for $j\lambda$ and an error δ, for the uncle Hamiltonian for the corresponding finite size chain, and for every $N \geq N_0$. The respective normalized vectors are also approximated eigenvectors for the same values, and therefore satisfy the statement in the lemma. □

However, these $j\lambda$ need not be in the spectrum, but indicate the existence of elements in the spectrum close to them, as it is shown in the following lemma.

LEMMA 5.4.17. *Let A be a self-adjoint operator on a finite dimensional Hilbert space, and λ a positive real value such that there exists a normal vector $|\varphi_{\lambda,\delta}\rangle$ with*

$$\|(A - \lambda\mathbb{I})|\varphi_{\lambda,\delta}\rangle\| < \delta.$$

Then $\sigma(A) \cap (\lambda - \delta, \lambda + \delta) \neq \varnothing$.

[28]Following the observation from eq. (48) at the end of the proof of Proposition 5.4.12.

PROOF. Let $\{\lambda_i\}_{i=1}^n$ be the set of eigenvalues (possibly repeated) of A, and $\{|\phi_i\rangle\}_{i=1}^n$ a corresponding orthonormal basis of eigenvectors. Then $|\varphi_{\lambda,\delta}\rangle$ can be writen as:

$$|\varphi_{\lambda,\delta}\rangle = \sum_{i=1}^{n} a_i|\phi_i\rangle,$$

and $A(|\varphi_{\lambda,\delta}\rangle) = \sum_{i=1}^n a_i\lambda_i|\phi_i\rangle$.

If $\sigma(A) \cap (\lambda - \delta, \lambda + \delta)$ were the empty set, we would have that

$$\|(A - \lambda\mathbb{I})|\varphi_{\lambda,\delta}\rangle\| = \|\sum_{i=1}^{n} a_i(\lambda_i - \lambda)|\phi_i\rangle\| > \|\sum_{i=1}^{n} a_i\delta|\phi_i\rangle\| = \delta,$$

which contradicts the conditions of the lemma. □

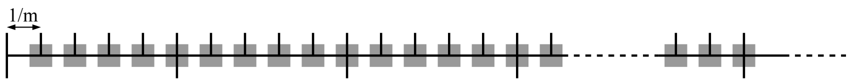
We have now all the ingredients we need to prove the main result of this chapter. Note that to reach this point we have needed to consider infinite systems and thermodynamic limits as tools to prove this result on finite size chains.

THEOREM 5.4.18. *The spectra of the uncle Hamiltonians for finite size chains tend to be dense in the positive real line for almost every perturbation P.*

PROOF. For any given values $L, m \in \mathbb{N}$, we can set

$$n = Lm, \ \ \lambda = 1/m \text{ and } \delta = 1/3m.$$

For these values, approximated eigenvectors can be found following Lemma 5.4.16, which indicate, due to Lemma 5.4.17, that $(j\lambda - \delta, j\lambda + \delta) \cap \sigma(H') \neq \varnothing$, $j = 1, \dots, n$, for every long enough chain. Therefore eigenvalues for every long enough chain can be found distributed in disjoint intervals centered on the set $j/m, j = 1, \dots, mL$ as depicted in the following diagram. These sets of eigenvalues, however possibly different for every chain length, tend to be dense in $\mathbb{R}^+$, as we consider higher values for L and m. □



5.5. Uncle Hamiltonians for injective spin chains.

As we have seen in Sec. 5.3.5, one can also construct interesting uncle Hamiltonians for injective MPS, if one chooses a non-canonical MPS representation of the state. To this end, let us start from an MPS $|M(A)\rangle$ with injective tensors A, and let

$$C = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}.$$

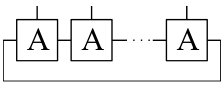
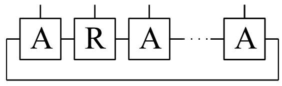
Then, $|M(C)\rangle = |M(A)\rangle$ denotes another MPS description of the same state. We can now consider a perturbation $C + \varepsilon \begin{pmatrix} P & R \\ R & P \end{pmatrix}$ and construct the corresponding uncle Hamiltonian H'.

Note that not any perturbation would lead to the same type of result. The tensor C has additional symmetries since both diagonal blocks are the same, and therefore we might get different results depending on the symmetries perturbation tensor shows. We will discuss on that issue later on in this section.

THEOREM 5.5.1. *Let A be the injective tensor description of a given MPS, and let us consider this MPS as described by the non-injective tensor*

$$\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}.$$

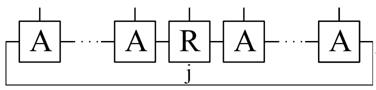
Given a perturbation tensor $C = \begin{pmatrix} P & R \\ R & P \end{pmatrix}$ *such that* $\begin{pmatrix} A & R \end{pmatrix}$ *is injective, the ground space of the uncle Hamiltonian H' for finite chains is spanned by*

 and $\sum_{\text{pos R}}$  .

This uncle Hamiltonian is local, frustration free, and gapless. The spectra of the finite chains tend to be dense in $\mathbb{R}^+$. In the thermodynamic limit the ground space collapses to a one-dimensional space[29]*, which is exactly the ground space of the thermodynamic limit of the parent Hamiltonian, and the spectrum is the whole positive real line $\mathbb{R}^+$.*

One can check this result following essentially the steps from the preceeding sections.

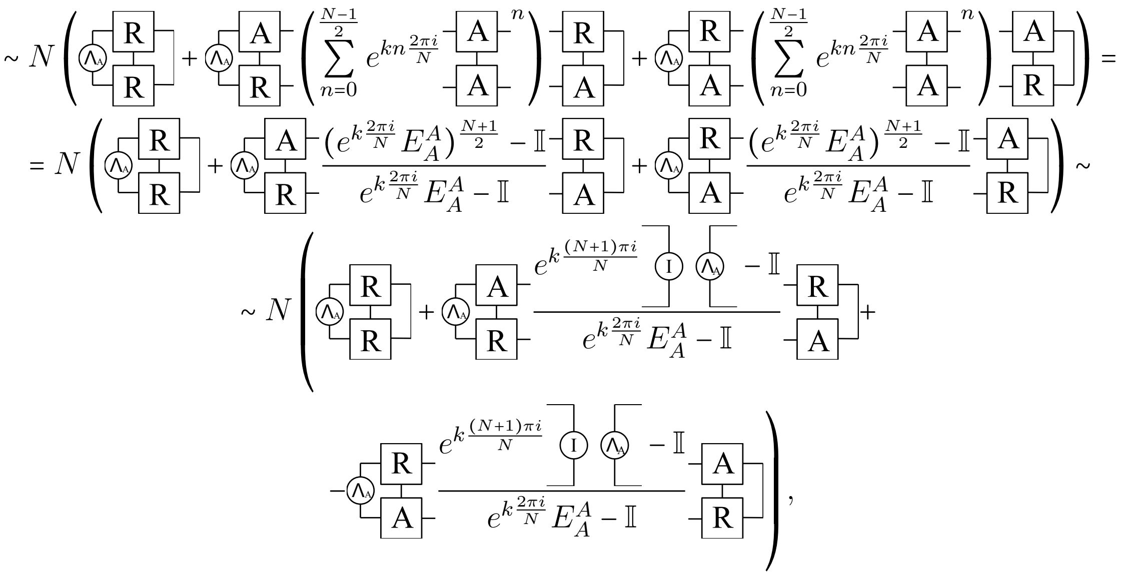
In a chain with length N, one can also consider as low energy states the states with momentum $|\varphi_k\rangle = \sum_j e^{2jk\pi i/N}|\zeta_j\rangle$, with

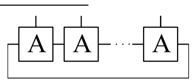
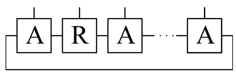
$|\zeta_j\rangle =$  .

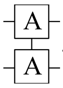
The calculations related to states with momentum can be reduced considerably, since $\langle\varphi_k|\varphi_k\rangle = Ne^{-2k\pi i/N}\langle\zeta^1|\varphi_k\rangle$ and $\langle\varphi_k|H'|\varphi_k\rangle = Ne^{-2k\pi i/N}\langle\zeta_1|H'|\varphi_k\rangle$.

When N is large enough (and odd), we can get the approximations

$$\langle\varphi_k|\varphi_k\rangle = Ne^{-k\frac{2\pi i}{N}}\langle\varphi^1|\varphi_k\rangle \sim$$

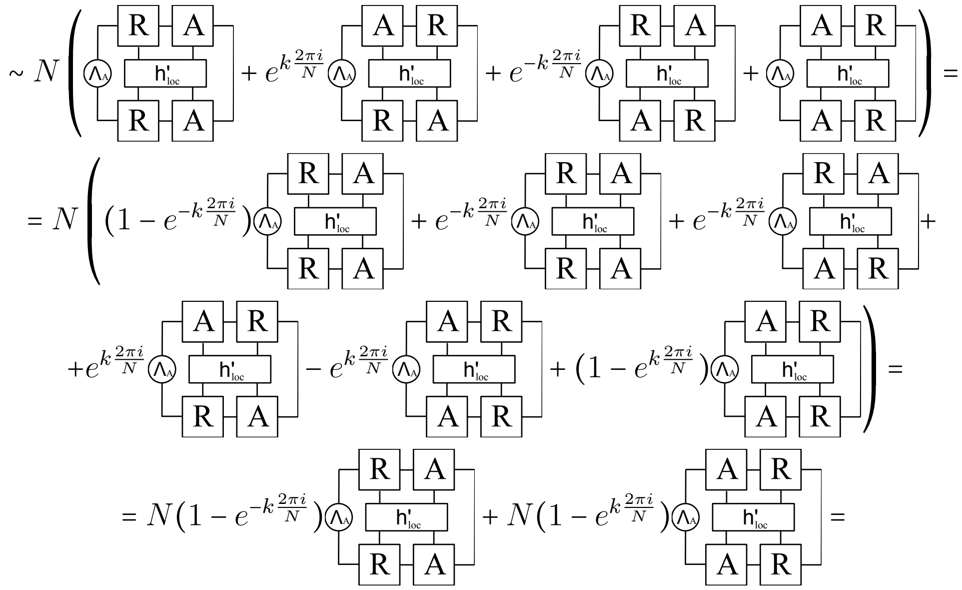


[29]  and $\sum_{\text{pos R}}$  lead to the same measurement statistics when the limit on infinite chains is considered.

where $E_A^A =$ . The expression multiplying N is either divergent or convergent to a constant different from 0 for almost every perturbation R. A similar result can be found for even values of N. Therefore, $\langle\varphi_k|\varphi_k\rangle = \Theta(N)$.

The value of $\langle\varphi_k|H'|\varphi_k\rangle$ can also be approximated as

$$\langle\varphi_k|H'|\varphi_k\rangle = e^{-k\frac{2\pi i}{N}}\langle\zeta_1|H'|\varphi_k\rangle = N\langle\zeta_1|H'(e^{-k\frac{2\pi i}{N}}|\zeta_N\rangle + |\zeta_1\rangle + e^{k\frac{2\pi i}{N}}|\zeta_2\rangle) \sim$$



$$= NO(\mathrm{Re}(1 - e^{k\frac{2\pi i}{N}})) = NO(1/N^2) = O(1/N)^{30}$$

.

The second equality is due to the fact that only two local Hamiltonians – those acting just on sites N, 1 and 2 – do not vanish. The equality from line 4 to line 5 above is due to span$\{A \overset{c}{-} R + R \overset{c}{-} A\}$ being contained in the kernel of h'_{loc}. Finally, note that the expression in line 2 – hence also expression in line 5 – is a real number, thus the equality from line 5 to line 6.

Hence, there can be found low energy states from this family of states. They are orthogonal to the ground space, and can be used to follow the steps in the previous sections in order to prove that the uncle Hamiltonian is gapless and its spectrum is $\mathbb{R}^+$ for some perturbations also for injective MPSs. It can be also proved that the spectra of finite size chains tend to be dense in $\mathbb{R}^+$ in this case.

Let us now comment what happens when blocks are not repeated in the chosen perturbation. Under a generic linear perturbation $\varepsilon\left(\begin{smallmatrix} P & R \\ L & Q \end{smallmatrix}\right)$, the local parent Hamiltonian in two sites would be

$$\Pi\begin{bmatrix} A \overset{c}{-} A + \varepsilon(A \overset{c}{-} P + P \overset{c}{-} A) + \varepsilon^2(P \overset{c}{-} P + L \overset{c}{-} R) & \varepsilon(A \overset{c}{-} L + L \overset{c}{-} A) + \varepsilon^2(P \overset{c}{-} L + L \overset{c}{-} Q) \\ \varepsilon(R \overset{c}{-} A + A \overset{c}{-} R) + \varepsilon^2(R \overset{c}{-} P + Q \overset{c}{-} R) & A \overset{c}{-} A + \varepsilon(A \overset{c}{-} Q + Q \overset{c}{-} A) + \varepsilon^2(L \overset{c}{-} R + Q \overset{c}{-} Q) \end{bmatrix},$$

[30]This bound also depends on k, as $O(k^2/N)$.

which equals

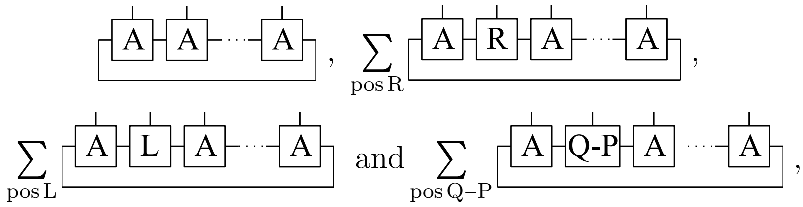
$$= \Pi \left[\begin{array}{cc} A\overset{c}{-}A + \varepsilon(A\overset{c}{-}P + P\overset{c}{-}A) + \varepsilon^2(P\overset{c}{-}P + L\overset{c}{-}R) & (A\overset{c}{-}L + L\overset{c}{-}A) + \varepsilon(P\overset{c}{-}L + L\overset{c}{-}Q) \\ (R\overset{c}{-}A + A\overset{c}{-}R) + \varepsilon(R\overset{c}{-}P + Q\overset{c}{-}R) & \begin{array}{c} (A\overset{c}{-}Q + Q\overset{c}{-}A - A\overset{c}{-}P - P\overset{c}{-}A) + \\ +\varepsilon(L\overset{c}{-}R + Q\overset{c}{-}Q - P\overset{c}{-}P - R\overset{c}{-}L) \end{array} \end{array} \right].$$

The second tensor can be obtained from the first by aplying the invertible map $\mathcal{L}_\varepsilon$ which multiplies the off-diagonal blocks by $1/\varepsilon$, and the map which sums the first diagonal block to the second diagonal block.

In such case, we would have to pay now attention to the new tensor

$$A\overset{c}{-}Q + Q\overset{c}{-}A - A\overset{c}{-}P - P\overset{c}{-}A$$

dominating the second diagonal block unless $P = Q$ (or slightly weaker assumptions). This tensor has a similar form to $A\overset{c}{-}L + L\overset{c}{-}A$, with $Q - P$ playing the role of L. Therefore, the only difference is that the ground state space would be spanned by



whenever $\begin{pmatrix} A & L \\ R & Q-P \end{pmatrix}$ is injective[31], which happens for almost every perturbation[32] .

[31]In the particular case $P = Q$, we would have to take the tensor $L\overset{c}{-}R - R\overset{c}{-}L$ into account, unless $R = L$. This would make the local kernel much larger, and the uncle Hamiltonians could show very different behaviours from those exposed, since we have not treated any similar case.

[32]Note that previous condition imposing $P = Q$ and $R = L$ in Theorem 5.5.1 made the perturbation lie on an algebraic variety, and therefore only a few perturbations satisfy that result as stated.

CHAPTER 6

Uncle Hamiltonian for the toric code.

The natural extension of Matrix Product States to higher dimensional lattices are the so-called Projected Entangled Pair States (PEPSs [**125**]). As Matrix Product States, they describe efficiently many interesting states – such as Resonating Valence Bond States [**116, 130**], cubic code [**51**], 2D cluster state [**125**] or 2D AKLT states [**1**] – and serve as framework for efficient numerical simulations, even though their perfomance in this setting is not that good.

One of the paradigmatic examples of PEPS in two dimensions is the one presented from Kitaev in [**67**]: the toric code. It was initially described as a stabilizer code, i.e. as the invariant subspace under some operators, over a toroidal lattice. For our purposes we describe it as a translationally invariant PEPS, with equivalent properties: 4-dimensional ground space and gapped parent Hamiltonian, local indistinguishability of ground states, automatic correction of local syndromes, topological corrections to entropy formulae, etc. These properties, some of which depend on the topological type of the lattice, are usually summarized under the name *topologial order*.

We use this important example to show that uncle Hamiltonians can also be found for non-injective higher dimensional tensor network states. Indeed, it was in a 2-dimensional honeycomb lattice model in which Chen et al. [**26**] noted that the parent Hamiltonian construction is not always robust under small variations of the tensor description, by studying the change of the topological entanglement entropy under variations of the tensor on a honeycomb lattice model.

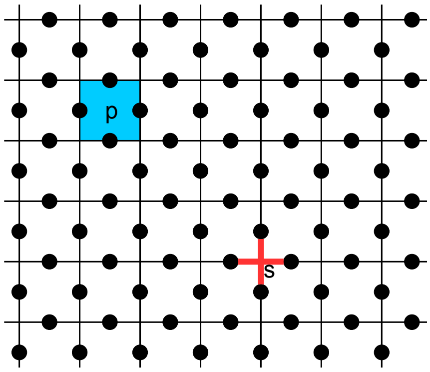
However, in opposition to the previous chapter related to MPSs, we do not construct the results in full generality. This is partly due to the fact that the theory of PEPS is not as well developed as the theory of MPSs, since there is no normal form for them.

6.1. Kitaev's toric code.

In this section we provide the description of the toric code originally proposed by Kitaev. We will afterwards work with a particular tensor description of this code.

Let us start with a 2-dimensional toroidal lattice of length k, with a 1/2-spin particle located at the middle point of every edge – that is, each site has physical dimension equal to 2. The full system $\mathcal{H}$ is equivalent to having $2k^2$ qubits, and therefore its dimension equals 2^{2k^2}.

We will consider two different types of interactions, the first one among the four particles surrounding a plaquette and the second one among the four particles connected to a vertex (or star). Plaquettes and stars are indicated in the picture with their initials p and s.



We will denote that a given site j is surrounding a plaquette p by $j \in \text{boundary}(p)$, and $j \in \text{star}(s)$ will denote that site j is connected to vertex s.

For every vertex s in the lattice, we consider the star operator

$$A_s = \Pi_{j\in \text{star}(s)} \sigma_j^x,$$

where $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and the subindex denotes at which site it is acting. For every plaquette p we consider the plaquette operator

$$B_p = \Pi_{j\in \text{boundary}(p)} \sigma_j^z$$

where $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Note these operators commute with each other, because the operators σ^x and σ^z anticommute when acting on the same site, and a plaquette and a star can have either 0 or 2 common edges. The operators A_s and B_p are Hermitian and have eigenvalues 1 and −1.

With this operators we can define the toric code Hamiltonian:

$$H = -\sum_s A_s - \sum_p B_p,$$

where the sums run over all the plaquettes p and all the stars s in the lattice.

The ground space of H is the *protected* subspace

$$\{|\varphi\rangle \in \mathcal{H},\ A_s|\varphi\rangle = |\varphi\rangle \text{ and } B_p|\varphi\rangle = |\varphi\rangle\ \forall s, p\},$$

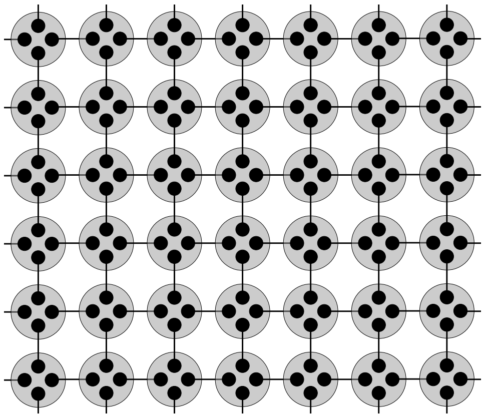
which is a 4-dimensional subspace of $\mathcal{H}$. This ground space is what is called toric code.

6.2. Projected Entangled Pair States and parent Hamiltonians.

Projected Entanged Pair States, as it happens for MPSs, are a family of states which satisfy the area law for the entanglement entropy. They are a powerful tool for both numerical and theoretical problems, since they are computationally tractable, and they provide new models with very interesting properties.

We will only consider 2D square toroidal. The generalization of PEPSs to higher dimensions or other lattices is straightforward. For simplicity, and because we will need no more in this chapter, we will also restrict the construction to translationally invariant PEPS.

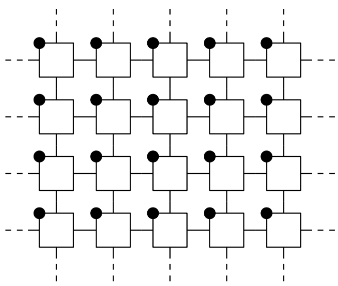
Let us start, as we did with MPSs, with the lattice and maximally entangled pairs $|\phi_{j,k}\rangle = \sum_{i=1}^{D} |ii\rangle$ located along every interacting bond (j,k) connecting two neighbouring sites, leading to the global state $|\Phi\rangle = \otimes_{(j,k)}|\phi_j\rangle$. D will be called the bond dimension.



We then apply a linear map $A : \otimes_4 \mathbb{C}^D \to \mathbb{C}^d$ to the four particles located at every vertex, each of them from an interacting bond, to get the PEPS associated to the map A:

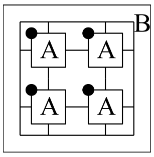
$$|P(A)\rangle = \otimes_j A|\Phi\rangle.$$

This map A has a tensor description, which we will identify usually with the map, with a physical index and 4 virtual indices. And as expected, the graphical description of higher dimensional tensor network states is more complicated than the one for MPSs. In 2-dimensional lattices, the physical index – with dimension d – is represented as a dot on the tensor, as if a leg were pointing out of the piece of paper. Tensor contraction is represented by joining legs.



A parent Hamiltonian can be always constructed for PEPS. However, it does not always have the good properties it exhibits in the case of MPSs. For some specific cases – injective, G-injective, isometric and G-isometric – some properties can be proven. Let us briefly introduce some of them.

Whenever the map A is injective the corresponding tensor is also called injective. In this case a parent Hamiltonian, with the corresponding PEPS as unique ground state, can be constructed for the full lattice considering local projections h_{loc} at every 2×2 region onto the orthogonal complement of the range of A as a map. This space will be described graphically as

$\ker h_{\text{loc}} = \Big\{$  $, B$ boundary condition $\Big\}$.

Following the notation used in the previous chapter in Section 5.1.4, this space is span$\{\overline{A}\}$ for $\overline{A}$ the tensor corresponding to the contraction of four copies of the A tensor as indicated above[1], and the local Hamiltonian is $h_{\text{loc}} = \Pi[\overline{A}]$. The tensor corresponding to the contraction of copies of an A tensor along a $n \times m$ region will be denoted by $\overline{A}^{(m,n)}$, with no superscript if $n = 2 = m$ as indicated before.

By summing these local projectors acting on every 2×2 region, we can construct the global parent Hamiltonian: $H = \sum h_{\text{loc}}$. The ground space of this parent Hamiltonian is the intersection of the kernels of the local projectors, and it is spanned by the PEPS associated to the tensor A, since we are supposing now A is injective [**100, 114**]. However, we cannot assure that this Hamiltonian is gapped.

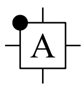
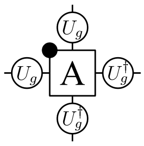
Note that injectivity is a very generic condition for a PEPS provided that the physical dimension d is greater that the virtual dimension D^4.

In the case the map A is not only injective but also isometric the tensor is also called isometric. In this case the Hamiltonian can be proven to be gapped.

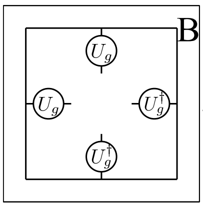
There is another family of PEPS for which parent Hamiltonians have some good properties: G-injective PEPS.

DEFINITION 6.2.1. Let $g \mapsto U_g$ be a unitary semirregular representation of a group G. A PEPS tensor A is called G-injective (resp. G-isometric) if the following two conditions hold:

i) A is invariant under U_g on the virtual level,

 $=$  $, \ \forall g \in G$

ii) A is injective (resp. isometric) when restricted to the subspace of U_g-invariant boundary conditions

$\left\{ \sum_{g \in G} \right.$  $\left., \ B \in \otimes_4 \mathbb{C}^D \right\}$

.

For G-injective PEPS, the ground space of the parent Hamiltonian – constructed also with local projectors on 2×2 regions – is degenerate. Its dimension equals the number of

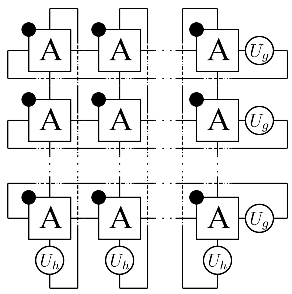
[1]We will use this notation in this chapter for this purpose.

'pair congujacy classes' of $G \times G$, determined by the equivalence relation

$$(g,h) \sim (g',h') \iff \exists x \in G,\ (g,h) = (xg'x^{-1}, xh'x^{-1}).$$

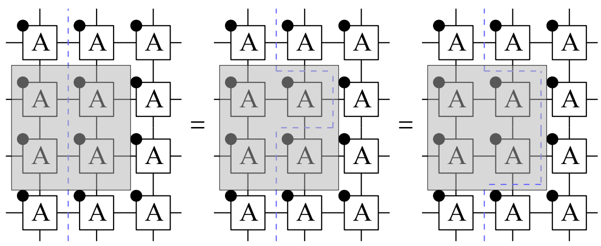
If the PEPS is also G-isometric the local Hamiltonians can be taken mutually commuting, and the parent Hamiltonian is gapped.

In the case of G-injective – and G-isometric – PEPS, the ground space is spanned by the family of states

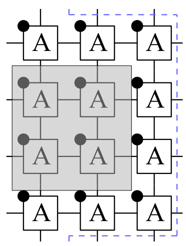
(49)  ,

where the boundary closures U_g and U_h depend on the different pair congujacy classes $[(g,h)]$.

The reason why these states appear in the ground space is the U_g-symmetry of the tensors, since the U_g and the U_h closures can be 'moved' to a different loop so that the local Hamiltonians cannot 'detect' them. For matrices U_g along the vertical bonds crossing the dotted loops in the figure, and U_g and $U_g^\dagger$ matrices suitably placed along the horizontal bonds also crossing the dotted loops, the following tensors are the same:



Thus, for a local Hamiltonian acting on the grey region, in the third case it can be seen that the U_g matrices do not prevent the state from being projected to 0, since this would imply just a different boundary condition for the region. The loop could be moved even further to



Note that the loop must be closed, since for U_g matrices placed along an open string the ends of the strings would be detected by a local Hamiltonian.

Remark 6.2.2. Block-injective MPSs are $\mathbb{Z}_n$-injective tensors, where n is the number of blocks of the tensor. The representation would be determined in this case by

$$1 \mapsto \oplus_j \eta^j \mathbb{I}_{l_j},$$

where η is a primitive n^{th}-root of 1.

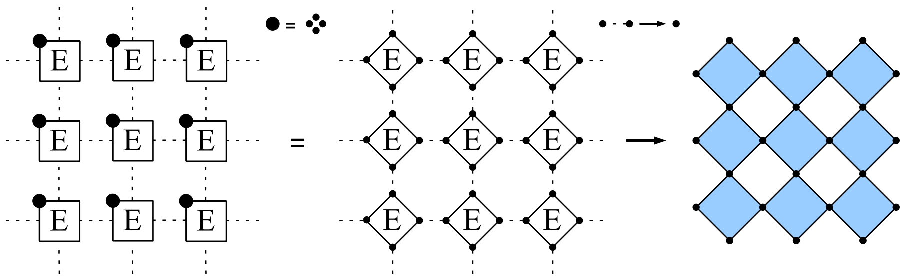
6.3. The toric code as a PEPS and its parent Hamiltonian.

In order to construct the toric code as a PEPS we can consider $\mathbb{C}^d = \otimes_4 \mathbb{C}^2$ as physical space at every site, and every bond having dimension two. The tensor E we will consider at every site is the orthogonal projection from the physical space onto the space of even spin configurations in the virtual space,

$$E|ijkl\rangle = \frac{1 + (-1)^{i+j+k+l}}{2} |ijkl\rangle.$$

This tensor is $\mathbb{Z}_2$-isometric, with respecto to the representation $U_1 = \sigma^z$ and $U_0 = \mathbb{I}$.

An easy way to relate this tensor network to the usual Kitaev's toric code description is to consider the graphs in next figure. On the left we have the PEPS description of the toric code. The rhombi in the middle term are just E tensors to which we cut the corners in the drawings, in order to make clearer the equivalence we will just explain. We also split the physical space at every site, which is $\otimes_4 \mathbb{C}^2$.

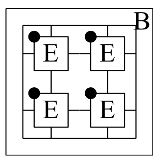


On the right, we have an alternative representation of the original toric code, with qubits in the vertices, and with coloured regions corresponding to plaquettes and white regions to stars. E rombhi map to coloured rombhi.

First note that $E = (\mathbb{I} - B)/2$, so for a vector on the right-hand the conditions $B|\varphi\rangle = |\varphi\rangle$ and $E|\varphi\rangle = 0$ are equivalent. Therefore, if at each bond we project $|ii\rangle \to |i\rangle$ – this projection commutes with the E projections – we get that the PEPS $P(E)$ is in the toric code protected space. Plaquette conditions are satisfied because of having applied E tensors, and star conditions are satisfied due to the a priori choice of maximally entangled states at the connecting bonds.

Other three independent generators of the code can be constructed by choosing, in the PEPS description, one column of bonds, one row of bonds, or both one column and one row, and then setting a σ^z operator at every selected bond.

These states are also generators of the ground space of the parent Hamiltonian for the PEPS, as described in eq. (49), which is constructed as the sum over every 2×2 square sublattice of the projection h_{loc} onto the orthogonal complement of E_{22} – that is, $\ker h_{\text{loc}} = E_{22}$ –, where

(50) $E_{22} = \Big\{$  , B boundary condition $\Big\}$

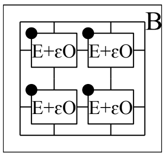
Recall that tensor E is $\mathbb{Z}_2$-isometric, and its parent Hamiltonian shows a spectral gap for increasing size regions. We must also say that we will not only consider $k \times k$ lattices. The toric code can be equally constructed for $k_1 \times k_2$ lattices, as well as this PEPS description for it. This will turn important when we try to construct the thermodynamic limit when we let one of the dimensions of the lattice grow while we keep the other one fixed.

6.4. Uncle Hamiltonian for the toric code.

Let us now derive the uncle Hamiltonian for the toric code, for an $N \times M$ lattice. This is done as for the GHZ state and MPSs: We perturb the toric code tensors, derive the corresponding parent Hamiltonian, and take the limit as the perturbation vanishes. In this case we consider only a specific perturbation, which we denote by O and is the complementary projection to E, $O = \mathbb{I} - E$. O is the projection onto the space of odd spin configurations:

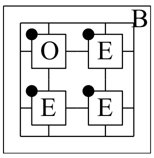
$$O|ijkl\rangle = \frac{1 + (-1)^{i+j+k+l+1}}{2}|ijkl\rangle.$$

The 2×2-site perturbed local Hamiltonian $h^{\varepsilon}_{\text{loc}}$ is

$h^{\varepsilon}_{\text{loc}} = \Pi[\overline{E + \varepsilon O}]$, that is, $\ker h^{\varepsilon}_{\text{loc}} = \Big\{$ 

, B boundary condition$\Big\}$.

In the limit when ε vanishes, we obtain a new projector, $h'_{\text{loc}} = \lim_{\varepsilon\to 0} h^{\varepsilon}_{\text{loc}}$, which is different from the local projector h_{loc} we started with: The new local Hamiltonian h'_{loc} is the projector onto the orthogonal complement of $E_{22} \oplus O_{22} = \ker h'_{\text{loc}}$, where

(51) $O_{22} = \Big\{ \sum_{\text{pos } O}$ 

, B boundary condition$\Big\}$,

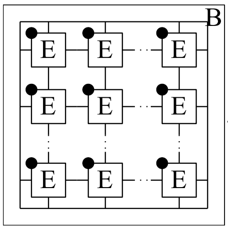
and this last sum runs over the positions which the single O tensor above may occupy among the four tensors appearing.

Note that, for product boundary conditions, vectors in E_{22} will only be non-zero for even parity boundary conditions B, whereas for O_{22} this will only be the case for odd boundary conditions.

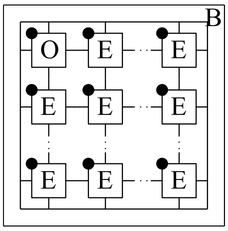
The new uncle Hamiltonian H' is constructed again as the sum over all 2×2 regions of the local projector h'_{loc}. When considering an $n \times m$ contractible region R, and the sum of the local projectors are acting entirely in this region, one finds that the kernel of this sum has the same structure as the kernel of a single projector:

$$\ker\Big(\sum_R h'_{\text{loc}}\Big) = \bigcap_R \ker h'_{\text{loc}} = E_{n,m} \oplus O_{n,m} = S_{n,m} \ ,$$

with definitions for $E_{n,m}$ and $O_{n,m}$ similar to eq. (50) and eq. (51) for $n \times m$ contractible regions:

$E_{n,m} = \Big\{ |\varphi_{E_{n,m}(B)}\rangle =$ 

$, B$ boundary condition$\Big\}$, and

$O_{n,m} = \Big\{ |\varphi_{O_{n,m}(B)}\rangle = \sum_{\text{pos}\, O}$ 

$, B$ boundary condition $\Big\}$.

We shall prove that fact, called *intersection property*, inductively using Proposition 6.4.1.

However, as we show in Proposition 6.4.2, the O summand disappears when imposing periodic boundary conditions to the full $N \times M$ lattice, and the ground space of the uncle Hamiltonian is exactly the same as the ground space of the parent Hamiltonian.

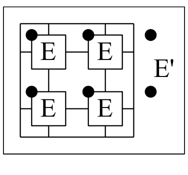
The space E_{22} plays the role span$\{|000\rangle, |111\rangle\}$ did in the uncle Hamiltonian for the GHZ state, and O_{22} plays the role of span$\{|0+1\rangle, |1+0\rangle\}$. There was no way to obtain periodic boundary condition with just one 'domain wall' – a 0 to 1 or 1 to 0 'delocalized' boundary– and the same will happen now for a unique O projector appearing in the tensor configuration. The same way two 'domain walls' were not allowed to appear in the ground state because they were not allowed to meet without any energy cost and they were the basis to obtain low energy states, now this situation is going to happen again for two delocalized O projectors appearing in the tensor configuration.

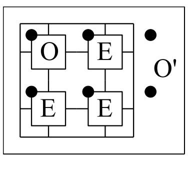
Hence, let us first prove that the intersection of the kernels of the h'_{loc} is indeed described by $S_{n,m}$. The following proposition serves as the first step for an induction process over n and m.

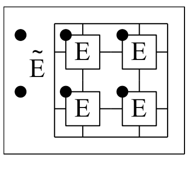
PROPOSITION 6.4.1 (Intersection property). Given a 2×3 lattice,

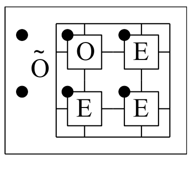
$$S_{22} \otimes \mathbb{C}^{2^8} \cap \mathbb{C}^{2^8} \otimes S_{22} = S_{23}.$$

PROOF. Let $|\phi\rangle$ be an unnormalized vector in $S_{22} \otimes \mathbb{C}^{2^8} \cap \mathbb{C}^{2^8} \otimes S_{22}$. This vector can be written in two different ways:

(52) $|\phi\rangle =$ 

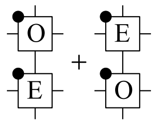
$+ \sum_{\text{pos}\, O}$ 

$=$ 

$+ \sum_{\text{pos}\, O}$ 

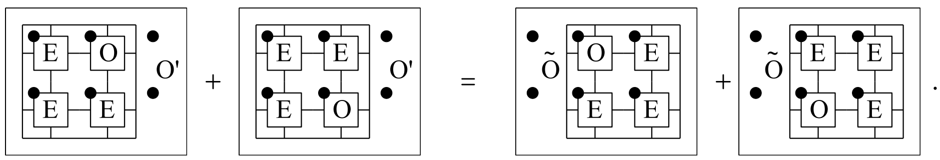
W.l.o.g. we can assume that the boundary conditions given by E' and $\tilde{E}$ are always even, and those given by O' and $\tilde{O}$ are always odd.

We can now perform the projection

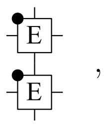


on the physical levels in the second column. As projections E and O are orthogonal, this last operation exactly selects this pattern in the second column, and we obtain the equality

(53)

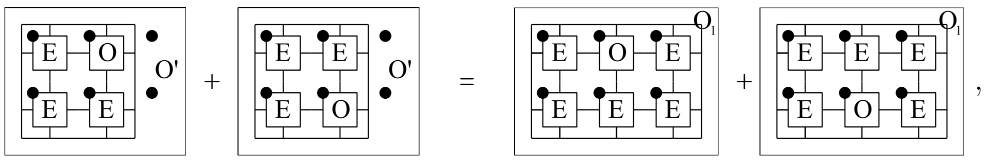


In order to infer the structure of O' and $\tilde{O}$, we project either the first or the third column onto



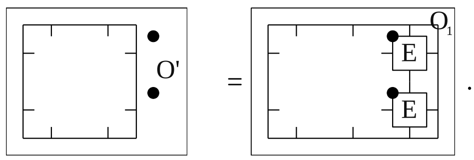
and use the fact that *i)* O' and $\tilde{O}$ have odd parity and *ii)* the resulting tensor network of E's and O's is equivalent to a projection onto the odd parity subspace.

By projecting at the first column, we find that there should exist some odd spain parity boundary condition O_1 such that



and therefore deduce

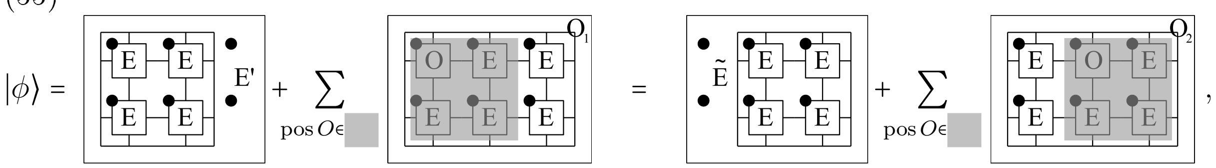
(54)



By projecting at the third column, we obtain the corresponding equation for $\tilde{O}$ with a boundary O_2. Re-substituting in (53), we find that $O_1 = O_2$, and this new boundary condition has odd parity.

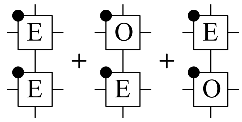
Substituting eq. (54) and its analog for $\tilde{O}$ back into eq. (52), we obtain

(55)

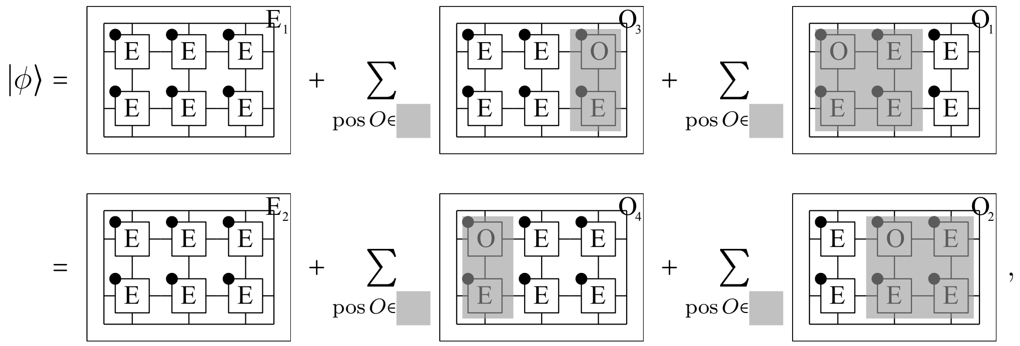


where the sums run over all positions of the O tensor inside the respective grey regions.

We now use the same trick to also infer the structure of E' and $\tilde{E}$: We apply the projection



in either the first or the third column of eq. (55); after re-substituting the resulting conditions, we find that



for some even parity boundary conditions E_1 and E_2, and some odd parity boundary conditions O_3 and O_4.

Finally, by matching equal patterns of E's and O's we can easily check that $E_1 = E_2$, $O_1 = O_4$, and $O_2 = O_3$. Thus, there exist unique even and odd boundary conditions $B_E = E_1 = E_2$ and $B_O = O_1 = O_2 = O_3 = O_4$ which describe the state $|\phi\rangle$ as an element from S_{23}. □

Using this argument inductively, we can indeed prove for any contractible rectangle of size $n \times m$ that $S_{n,m}$ is equal to the intersection of the kernels of the local Hamiltonians h'_{loc} which act entirely inside the region.

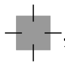
Let us now consider the whole lattice with periodic boundary conditions, and study the ground state space of the global uncle Hamiltonian.

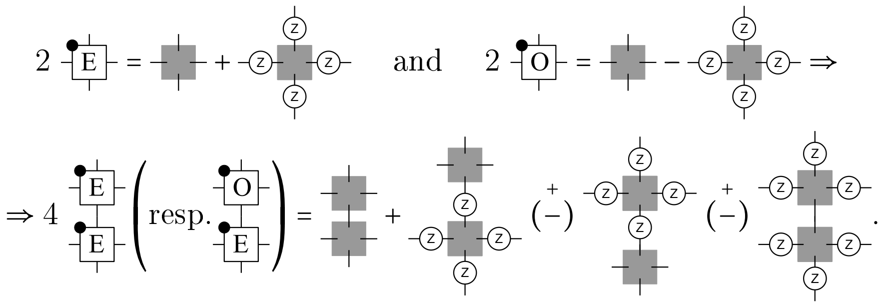
Proposition 6.4.2 (Closure property). The ground space of the uncle Hamiltonian coincides with the ground space of the parent Hamiltonian.

Proof. Exploiting the σ^z symmetry of E and O tensors, we can prove that for a state to lie in the kernel of every h'_{loc}, and therefore in the kernel of H', it should remain invariant under the projection at any two sites connected by any bond onto

$$\operatorname{span}\{|00\rangle + |11\rangle, |0\rangle\sigma^z(|0\rangle) + |1\rangle\sigma^z(|1\rangle)\} = \operatorname{span}\{|00\rangle, |11\rangle\}.$$

Let us show why.

If we denote the identity by , and setting $Z = \sigma^z$, we have



First and last summands in this last expression remain invariant under projection onto span$\{|00\rangle + |11\rangle\}$ at the sites conected by the bond, and second and third summands under projection onto span$\{|0\rangle \otimes \sigma^z(|0\rangle) + |1\rangle \otimes \sigma^z(|1\rangle)\}$ = span$\{|00\rangle - |11\rangle\}$. Therefore, if we project onto the sum of these two spaces the tensors remains unchanged.

Thus only linear combinations of the identity and σ^z may appear in the closure bonds when imposing periodic boundary conditions, and all periodic boundary conditions are necesarily even. Hence, given the full lattice and periodic boundary conditions, the elements in S_{NM} which came from O_{NM} cannot be in the kernel of the global uncle Hamiltonian.

Consequently S_{final}, the ground space of the uncle Hamiltonian, is constructed by imposing periodic boundary conditions to E_{NM}, and therefore coincides with the ground state subspace of the toric code parent Hamiltonian, spanned by the states in eq. (49) and whose detailed construction can be found in [**114**]. □

6.5. Spectrum of the uncle Hamtiltonian for the toric code.

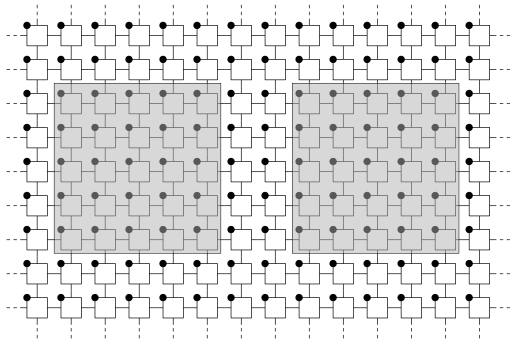
Let us now show that the uncle Hamiltonian for the toric code is gapless for size-growing finite lattices, and that its spectrum in the thermodynamic limit is the postive real line. Finally, we shall prove that the spectra of the uncle Hamiltononians on finite lattices tend to be dense in $\mathbb{R}^+$.

6.5.1. Gaplessness of the uncle Hamiltonian.

First, we consider the family of uncle Hamiltonians defined on finite size regions. The parent Hamiltonian can be easily shown to be gapped, since it consist of commuting local terms. On the contrary, the uncle Hamiltonian is gapless.

THEOREM 6.5.1. *The uncle Hamiltonian H' for the toric code is gapless.*

PROOF. As we did with the uncle Hamiltonian for the GHZ state, we consider a family of low energy states which are orthogonal to the ground space. Given any integer value of r, and for a lattice large enough, we may take two contractible rectangles R_1 and R_2 of size $r \times r$ which are separated by at least two columns. We construct a family of unnormalized states $|\phi_r\rangle$ by placing at these two regions the tensor spanning O_{rr} and setting all remaining tensors to E:

(56) $$|\phi_r\rangle = \sum_{\substack{\text{pos } O_1 \in R_1 \\ \text{pos } O_2 \in R_2}}$$  ,

with closed boundary conditions. That is, each of the grey regions contains exactly one O tensor and E's otherwise, and the sum runs over the possible positions of the two O's in each respective region.

These states are orthogonal to the ground space of the uncle Hamiltonian due to the orthogonality between tensors E and O.

The norm of all these summands is the same, say C. This value depends only on the total dimension of the lattice. Thus the norm of any of these $|\phi_r\rangle$ is Cr^2, since the summands are mutually orthogonal – due again to orthogonality between tensors E and O – and there are r^4 of them.

In order to compute $\langle\phi_r|H'|\phi_r\rangle$ we observe that only those local Hamiltonians h'_{loc} overlapping the boundary of these regions contribute a positive energy. There are only $8r$ of them, $4r$ overlapping the boundary of R_1 and $4r$ for R_2. For each of them at most $2r^2$ summands from (56) add any energy: there are at most two places where O can be located in the effective 2×2 region one of these local Hamiltonians is acting at, and the r^2 comes from all the different positions O may take in the other region – the one each of these local Hamiltonians does not overlap.

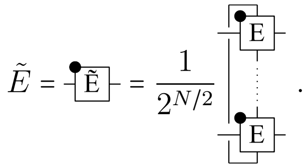
Hence $\langle\phi_r|H'|\phi_r\rangle = C^2\Theta(r^3)$, and the energy $\langle\phi_r|H'|\phi_r\rangle/\langle\phi_r|\phi_r\rangle$ of these states decreases as $O(1/r)$, independently of the lattice size. Altogether, this proves that H' is gapless. $\square$

6.5.2. Spectrum of the uncle Hamiltonian in the thermodynamic limit. We can now move to the thermodynamic limit of the uncle Hamiltonian on infinite lattices, and study its spectrum. We can consider one of the lattice dimensions fixed or none of them. In either case, we find that the uncle Hamiltonian is gapless in the thermodynamic limit and its spectrum is $\mathbb{R}^+$.

Thermodynamic limit with one of the dimensions of the lattice fixed. Let us first consider one of the dimensions of the system is fixed – let us choose the vertical one, set to the value N – and let the other go to infinity. We can block the tensors along the fixed dimension to reduce the problem to an MPS-like problem, but note that the parent and uncle Hamiltonians for the PEPS description are not parent nor uncle for the MPS description.

Let $\tilde{E}$ be the MPS tensor

(57)

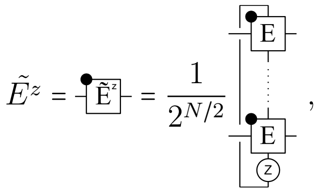


This tensor is a 2-block injective MPS tensor in its normal form, with blocks

for $\Pi_E : \otimes_N \mathbb{C}^2 \to E(\otimes_N C^2)$ the projector onto the subspace of even parity spin configurations, and $\Pi_O : \otimes_N \mathbb{C}^2 \to O(\otimes_N C^2)$ the projector onto the subspace of odd parity spin configurations. The multiplicative constant added in the definition of $\tilde{E}$ already makes this two blocks be in their normal form. The left fixed point for both blocks is proportional to the identity matrix:

$$\Lambda_{\tilde{E}_O} = \frac{1}{2^{N-1}} \mathbb{I}_{2^{N-1}} = \frac{1}{2^{N-1}} \mathbb{I}_{E(\otimes_N C^2)} \text{ and } \Lambda_{\tilde{E}_E} = \frac{1}{2^{N-1}} \mathbb{I}_{2^{N-1}} = \frac{1}{2^{N-1}} \mathbb{I}_{O(\otimes_N C^2)} \ .$$

Let us also define $\tilde{E}^z$ as the MPS tensor



and analogue definitions for $\tilde{E}^z_E$ and $\tilde{E}^z_O$ as those before.

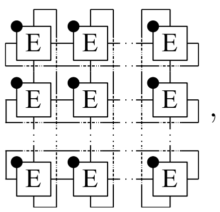
Then the limit[2] of the ground states for both the parent and the uncle Hamiltonian for the toric code, with periodic boundary conditions along the columns and open boundary conditions along the rows, are convex combinations of the thermodynamic limit states

$$\omega_{\tilde{E}_E} \ , \ \omega_{\tilde{E}_O} \ , \ \omega_{\tilde{E}^z_E} \ \text{ and } \ \omega_{\tilde{E}^z_O} \ .$$

Let us take as base ground state for the GNS-representation the state

$$\omega = (\omega_{\tilde{E}_E} + \omega_{\tilde{E}_O})/2,$$

which is the limit of the ground states of the form



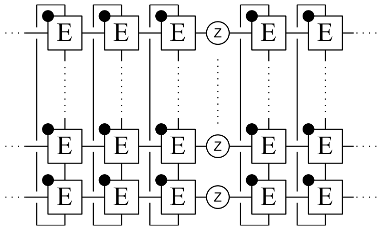
up to renormalization of the tensor E. In the following, the tensor E is the one we used along this section multiplied by a constant so that the limit is normalized. This new

[2]Recall from Section 5.4.4 that this is an informal statement. The limit we take in thermodynamic limit is that of the evolution determined by the interactions, and therefore the limit of the Hamiltonian.

constant[3] is

$$\sqrt[N]{\frac{1}{2^{(N+1)/2}}} = \frac{1}{\sqrt{2}\,\sqrt[2N]{2}}.$$

Note that ω is also the limit of states of the form



,

for the loop of σ^z operators can be moved far away from any local region, and therefore no local observable can be affected by this difference.

One could use a similar procedure to the calculations made in the previous chapter for MPSs to find the spectrum of this thermodynamic limit. However, one can also restrict the problem to a bounded operator as we did for the uncle Hamiltonian for the GHZ. Let us expose this last method.

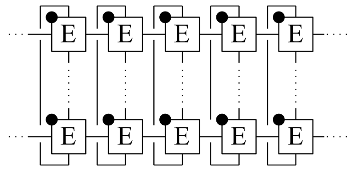
THEOREM 6.5.2. *The spectrum of the thermodynamic limit H'_ω of the uncle Hamiltonian for the toric code is the positive real line if we keep one of the lattice dimensions fixed.*

PROOF. First we take the GNS-representation with respect to the ground state

$$\omega = (\omega_{\tilde{E}_E} + \omega_{\tilde{E}_O})/2.$$

The distinguished cyclic vector for the representation can be represented as

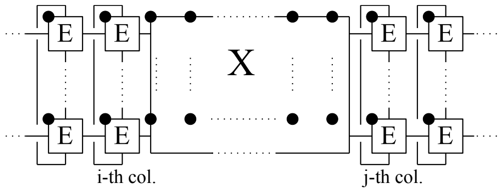
$$\Omega_\omega =$$



.

The details about the GNS-representation and why we can take such diagrams to describe the states in $\mathcal{H}_\omega$ can be found in the previous chapter, in sections 5.2.3 and 5.4.4. The thermodynamic limit of H' can be studied as acting on the completion of the vector space $S = \bigcup_{i<j} S_{i,j}$, where

$$S_{i,j} = \Big\{\phi_{i,j}(X) =$$



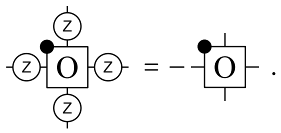
$$,\ X \text{ is } U_g\text{-symmetric}\Big\},$$

and X runs over all possible σ^z-symmetric tensors. We will usually omit the location of X whenever this does not matter due to translational invariance of the Hamiltonian.

[3]Note that this normalization constant is different from the one in equation 57. In this equation each block – $\tilde{E}_E$ and $\tilde{E}_O$ – is normalized separately, so that the corresponding limit states in the thermodynamic limit – $\omega_{\tilde{E}_E}$ and $\omega_{\tilde{E}_O}$ – are normalized states. Since we are taking now both blocks together, we get the same constant up to a factor $\sqrt{2}$. Without this factor we would get the unnormalized state $\omega = \omega_{\tilde{E}_E} + \omega_{\tilde{E}_O}$.

The Hamiltonian in the thermodynamic limit will be called H'_ω, as the unique self-adjoint extension of H' to $\mathcal{H}_\omega = \bar{S}$.

Contained in S we can find the space S^2 spanned by vectors with the tensor E everywhere but two places in which the tensor O is located – O is also considered renormalized as E. Note that



Therefore, locating two of such tensors can be expressed as a σ^z-symmetric tensor X. In the case these two copies of O are located in places (i,j) and (k,l) of the lattice, we call this state $|\phi_{i,j}^{k,l}\rangle$.

For each of these vectors, $H'(|\phi_{i,j}^{k,l}\rangle) \in \operatorname{span}\left\{|\phi_{i+\delta_i,j+\delta_j}^{k+\delta_k,l+\delta_l}\rangle,\ \delta_i,\delta_j,\delta_k,\delta_k \in \{-1,0,1\}\right\}$. Therefore, $H'(S^2) \subseteq S^2$. Moreover, $H'|_{S^2}$ is bounded[4], and consequently it can be uniquely extended to $\overline{S^2}$, coinciding on it with H'_ω.

Since the vertical dimension is now fixed – recall that its value is N – the regions used to construct the states $|\phi_r\rangle$ from (56) cannot grow indefinitely. We can consider instead similar unnormalized states $|\phi_{r,N}\rangle$, coming from $r \times N$ regions for growing values of r, embedded in S^2 to prove the existence of a sequence of elements in the spectrum $\{\lambda_i\}_{i=1}^\infty$ tending to 0.

For such spectral values, one can find Weyl sequences in $\overline{S^2}$ associated to them:

$$\frac{\| H'(|\varphi_{\lambda_i,j}\rangle) - \lambda_i |\varphi_{\lambda_i,j}\rangle \|}{\| |\varphi_{\lambda_i,j}\rangle \|} \xrightarrow{j\to\infty} 0.$$

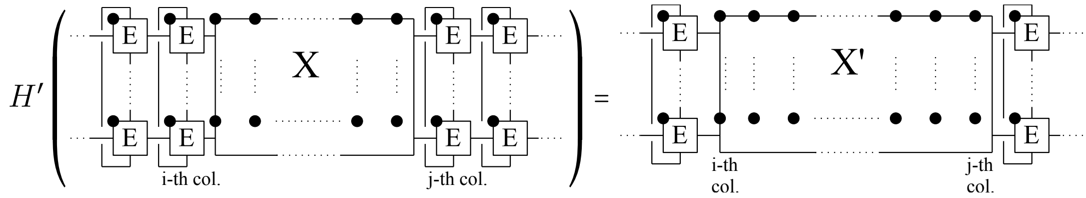
Using density arguments – as explained in the previous chapter for the GHZ state and MPSs – one can also find Weyl sequences lying in S^2 for the same values. Therefore, for any given λ_i and any $\delta > 0$ there must exist a – normalized – state $|\phi_{i,\delta}\rangle$ which is almost an eigenvector of H' for the value λ_i with an error at most δ , which means $\|(H' - \lambda_i \mathbb{I})|\phi_{i,\delta}\rangle\| \le \delta \| |\phi_{i,\delta}\rangle \| = \delta$.

If we write two – or more – of these states as $|\phi_{i_1,\delta_1}\rangle = |\phi(X_1)\rangle$ and $|\phi_{i_2,\delta_2}\rangle = |\phi(X_2)\rangle$, we can construct a new X by concatenating X_1 and X_2 separated by at least two columns of E tensors[5]. We can call $|\phi_2(X_1,X_2)\rangle$ such a vector – the subindex indicates how many columns with E tensors are between X_1 and X_2. This vector is an approximated eigenvector of H' for $\lambda_{i_1} + \lambda_{i_2}$ for an error at most $\delta_1 + \delta_2$. Let us prove that.

[4]The family $|\phi_{i,j}^{k,l}\rangle$ form a 1-symmetric basis of S^2, and we can proceed as in Lemma 5.3.2 in order to compute a bound.

[5]Two columns are enough because E is G-isometric. For isometric MPSs the calculations in Lemma 5.1.8 do not need the exponential correction for two or more copies of the transfer operator.

The first thing we need to note is that for any $|\phi(X)\rangle$ there exists a tensor X' such that $H'(|\phi_{i,j}(X)\rangle) = |\phi_{i-1,j+1}(X')\rangle$



The second fact we use is that, if X and X' have been chosen properly to make $|\phi(X_1)\rangle$ and $|\phi(X_2)\rangle$ have norm equal to 1, then the norm of $|\phi_2(X_1, X_2)\rangle$ is also 1. This is thanks to the specific structure of the tensor E. We have also that the norms of $|\phi_1(X_1', X_2)\rangle$ and $|\phi_1(X_1, X_2')\rangle$ are respectively equal to the norms of $|\phi(X_1')\rangle$ and $|\phi(X_2')\rangle$.

Hence, due to the locality of H', we have that

$$H'(|\phi_2(X_1, X_2)\rangle) = |\phi_1(X_1', X_2)\rangle + |\phi_1(X_1, X_2')\rangle \overset{\delta_1+\delta_2}{\sim}$$

$$\overset{\delta_1+\delta_2}{\sim} \lambda_{i_1}|\phi_2(X_1, X_2)\rangle + \lambda_{i_2}|\phi_2(X_1, X_2)\rangle = (\lambda_{i_1} + \lambda_{i_2})|\phi_2(X_1, X_2)\rangle.$$

Recall that the approximation above means

$$\|H'(|\phi_2(X_1, X_2)\rangle) - (\lambda_{i_1} + \lambda_{i_2})|\phi_2(X_1, X_2)\rangle\| \le \delta_1 + \delta_2.$$

Consequently, we can find a Weyl sequence for $\lambda_1 + \lambda_2$, which lies in the spectrum of the thermodynamic limit. For any finite sum of spectral values we can proceed in a similar way.

This family of vectors let us see that any finite sum of λ_i lies in the spectrum of H'_ω. The set of finite sums of a sequence of elements tending to 0 is dense in the positive real line, and the spectrum is closed, hence $\sigma(H'_\omega) = \mathbb{R}^+$. □

Thermodynamic limit with no lattice dimension fixed. When both dimensions are allowed to grow, the themodynamic limits of both parent and uncle Hamiltonians have a unique ground state,

$$\omega(A) = \frac{\sum_i \langle \varphi_{E_{n,m}(B_i)}|A|\varphi_{E_{n,m}(B_i)}\rangle}{\sum_i \langle \varphi_{E_{n,m}(B_i)}|\varphi_{E_{n,m}(B_i)}\rangle} = \frac{\operatorname{tr}\left(\overline{E}^{(n,m)^*} A \overline{E}^{(n,m)}\right)}{\operatorname{tr}\left(\overline{E}^{(n,m)^*} \overline{E}^{(n,m)}\right)}, \tag{58}$$

for a local observable A acting on a $n \times m$ region R and $\{|B_i\rangle\}_i$ any orthonormal basis of the space of all possible even parity boundary conditions[6] of $E_{n,m}$, and continously extended to the entire algebra of quasi-local observables.

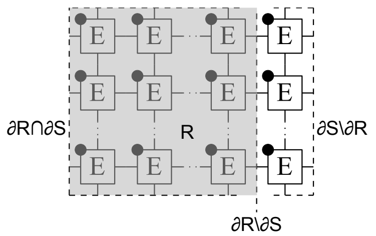
The state ω is well defined on the algebra of local observables, let us prove it.

Let $S \supset R$ be the $n \times (m+1)$ region resulting from adjoining a column to R, and let $\{B_i\}_i$ and $\{B_j'\}_j$ be the product bases of the spaces of even parity boundary conditions of $E_{n,m}$ and $E_{n,m+1}$ respectively. For any boundary condition B_j', there is a subset of the first basis $\{B_i\}_{i\in I_j}$ such that B_j' coincides with every B_i of this subset along the common boundary $\delta R \cap \delta S$ of R and S. Note that for two different B_j' and $B_{j'}'$ we can have either

[6]Recall that $|\varphi_{E_{n,m}(B)}\rangle = 0$ for every odd parity boundary condition B.

$I_j = I_{j'}$ – in the case B'_j and $B'_{j'}$ coincide along $\delta R \cap \delta S$ – or $I_j \cap I_{j'} = \varnothing$. We also have that $|I_j| = 2^{n-1}$ for every j, and that for every j the number of different $B'_{j'}$ leading to the same I_j is

$$|\{j',\ I_{j'} = I_j\}| = 2^{n+1}\,.$$



For every B'_j and B_i, $i \in I_j$, there exists a normal vector $|\psi_{i,j}\rangle$ in the physical space of the region $S\backslash R$ such that

$$|\varphi_{E_{n,m+1}(B'_j)}\rangle = \sum_{i \in I_j} |\psi_{i,j}\rangle \otimes |\varphi_{E_{n,m}(B_i)}\rangle\ ,$$

and $\langle\psi_{i,j}|\psi_{k,j}\rangle = \delta_{i,k}$.

Therefore we have

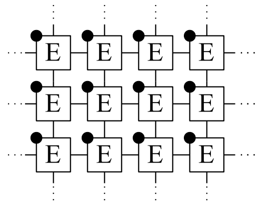
$$\begin{aligned}
\frac{\sum_j \langle\varphi_{E_{n,m+1}(B'_j)}|A \otimes \mathbb{I}_{S\backslash R}|\varphi_{E_{n,m+1}(B'_j)}\rangle}{\sum_j \langle\varphi_{E_{n,m+1}(B'_j)}|\varphi_{E_{n,m+1}(B'_j)}\rangle} &= \frac{\sum_j \sum_{i,k\in I_j} \big(\langle\psi_{i,j}| \otimes \langle\varphi_{E_{n,m}(B_i)}|\big)\, A \otimes \mathbb{I}_{S\backslash R} \big(|\psi_{k,j}\rangle \otimes |\varphi_{E_{n,m}(B_k)}\rangle\big)}{\sum_j \sum_{i,k\in I_j} \big(\langle\psi_{i,j}| \otimes \langle\varphi_{E_{n,m}(B_i)}|\big)\big(|\psi_{k,j}\rangle \otimes |\varphi_{E_{n,m}(B_k)}\rangle\big)} \\
&= \frac{\sum_j \sum_{i,k\in I_j} \langle\psi_{i,j}|\psi_{k,j}\rangle\langle\varphi_{E_{n,m}(B_i)}|A|\varphi_{E_{n,m}(B_k)}\rangle}{\sum_j \sum_{i,k\in I_j} \langle\psi_{i,j}|\psi_{k,j}\rangle\langle\varphi_{E_{n,m}(B_i)}|\varphi_{E_{n,m}(B_k)}\rangle} \\
&= \frac{\sum_j \sum_{i\in I_j} \langle\varphi_{E_{n,m}(B_i)}|A|\varphi_{E_{n,m}(B_i)}\rangle}{\sum_j \sum_{i\in I_j} \langle\varphi_{E_{n,m}(B_i)}|\varphi_{E_{n,m}(B_i)}\rangle} \\
&= \frac{2^{n+1} \sum_i \langle\varphi_{E_{n,m}(B_i)}|A|\varphi_{E_{n,m}(B_i)}\rangle}{2^{n+1} \sum_i \langle\varphi_{E_{n,m}(B_i)}|\varphi_{E_{n,m}(B_i)}\rangle}\ .
\end{aligned}$$

We may perform a similar calculation for a new region resulting from adjoining a row instead of a column. Therefore, one can inductively show that the definition of the state does not depend on the size of the region as long as the local observable is acting entirely within this region.

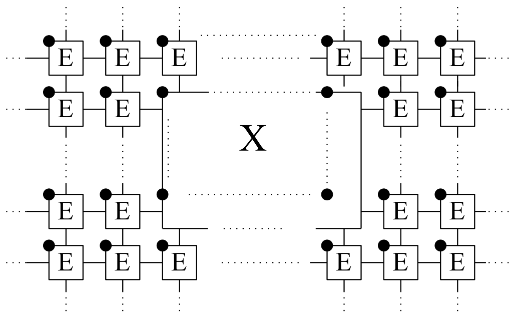
We cannot choose a constant C so that the tensor CE leads directly to a normalized version of the formula (58) without any quotient, because $\operatorname{tr}\left(\overline{E}^{(n,m)^*}\overline{E}^{(n,m)}\right) = 2^{nm+n+m}$, which is not of the form C^{nm} we would need for some C in order to be able to normalize in such a way.

The state ω is the limit of the states in the ground state space of both parent and uncle Hamiltonians with closed boundary conditions. This can be easily proven from the fact that closure conditions can be moven far apart from the region a local observable is effective on. In addition, it is also the limit of every state in both ground state spaces when open boundary conditions are considered: for the states in the spaces $O_{k,l}$, those summands for which no O tensor is located in the region a local observable is acting on lead to the same result as if no O tensor were present in the configuration, and this type of summands are clearly dominant[7] for increasing regions.

By taking the GNS-representation, we can describe the distinguished cyclic vector as

(59) $\Omega_\omega =$  .

The Hilbert space $\mathcal{H}_\omega$ we must consider is the completion of the linear space spanned by vectors of the type

$|\varphi(X)\rangle =$  ,

where X is the result of contracting some observable A_X acting on the lattice in (59) and the corresponding quotient should be taken into account. This implies that X must be σ^z-symmetric. The norm of such a vector can be calculated with the equation in (58) for the observable $A_X A_X^*$, by taking any region big enough such that X acts entirely on it.

Similar calculations to those from Section 6.5.1 show that the thermodynamic limit H'_ω of the uncle Hamiltonian is also gapless when no dimension is fixed.

We consider two regions R_1 and R_2 of size $r \times r$, For every $(i_1, j_1) \in R_1$ and $(i_2, j_2) \in R_2$, we consider the normalized vector $|\varphi_{i_1,j_1}^{i_2,j_2}\rangle$ consisting of placing an O tensor at these two sites in the net, up to a normalization constant. Note that this can be expressed as a U_g-invariant tensor X as required. Moreover, this can be achieved by acting on Ω_ω with a local unitary overlapping the two regions, and therefore any of these vectors has norm 1.

All the vectors just constructed are orthogonal to Ω_ω, and they are also mutually orthogonal. The rest of arguments from Section 6.5.1 are valid for the states

$$|\varphi_r\rangle = \sum_{\substack{(i_1,j_1)\in R_1 \\ (i_2,j_2)\in R_2}} |\varphi_{i_1,j_1}^{i_2,j_2}\rangle \ ,$$

bearing in mind that the constant in this case for every summand is $C = 1$. Therefore, the thermodynamic limit H'_ω is also gapless.

We can now proceed following the steps we took when we considered one of the dimensions fixed. The only difference is that, in this case, for the vectors in the Weyl sequences we need to find tensors X_i in bounded regions. Thus we get the result that the spectrum is also $\mathbb{R}^+$ in this case.

[7]With a ratio of the type $k^2 l^2$ versus $2klnm$, for an observable acting effectively on a $m \times n$ region and a lattice with dimension $k \times l$.

THEOREM 6.5.3. *The spectrum of the thermodynamic limit H'_ω of the uncle Hamiltonian for the toric code is the positive real line if we keep no lattice dimension fixed.*

6.5.3. Spectrum of the uncle Hamiltonian for finite lattices. We can now turn back to the study of spectra on finite lattices, and show that the spectrum is not only gapless, but it also tends to be dense in the positive real line as the lattice grows.

THEOREM 6.5.4. *The spectra of the uncle Hamiltonians for the toric code on finite size lattices tend to be dense in $\mathbb{R}^+$.*

PROOF. Following the steps we did for MPSs in the previous chapter, we can deduce that the finite sums $\sum_{i=1}^n \lambda_i$ of eigenvalues from the thermodynamic limit spectrum lie close to eigenvalues of the uncle Hamiltonian for large enough finite sized lattices, whether we keep one of the dimensions fixed or we let them both grow.

Tensors as X and X' in the previous section can be used to construct vectors in big enough finite dimensional lattices to this purpose.

Hence the spectra of the finite sized uncle Hamiltonians tend to be dense in $[0, \infty)$. $\square$

CHAPTER 7

Conclusions and future work.

Most of the conclusions have already been mentioned in the respective chapters, but let us summarize them now, together with questions and problems we would like to address in the future.

Rearrangement invariant structures in tensor products. Regarding the problem of state convertibility, we have found that symmetry and multiplicativity, together with majorization, are the only essential ingredients in order to characterize this task in the ELOCC and MLOCC settings. Mathematically, we have provided a characterization of ℓ_p spaces and c_0 among those spaces with symmetric bases based on mutiplicativity. We have also characterized L_p spaces among rearrangement invariant spaces as those satisfying an analogue multiplicative property.

We have shown that an analogue of Pisier-Schütt Theorem for spaces with symmetric bases cannot be obtained, by showing two examples that would contradict such result. However, one could think of strengthening the conditions on the crossnorm used for the tensor product: Could a Pisier-Schütt-type theorem exists for symmetric bases if we restrict to tensor norms? That is, for two spaces X and Y with symmetric bases, and $Z = X\hat{\otimes}_\alpha Y$ the completion of $X \otimes_\alpha Y$ for some tensor norm α, is it true that whenever Z has a symmetric basis the product basis is also symmetric? In such case, the results we have proven would yield that the only possibilites would be ℓ_1 and c_0, respectively with the projective and injective tensor norms: $\Delta_1 = \pi$ and ε.

It must be worth mentioning that our result and a later analogue one [**11**] motivated a posterior work by Leinster on a multiplicative characterization of the power means [**73**], which are the not necessarily positive analogues of the p-norms of the type $\sum_{i=1}^n x_i^p$, where different weights for the coordinates can be considered.

Coming back to the quantum setting, it would be very interesting studying the tripartite convertibility problem. Can some kind of symmetric structure be related to the LU characterization existing for this case, and can this structure be considered together with some order such that LOCC convertibility can be decided in the pure tripartite setting?

7.0.4. Joint measurability and Bell inequalities. In the problem of joint measurability, we have found a novel relationship between uncertantity and non-locality, two of the major consequences of Quantum Mechanics. This is not only a qualitative result, but also a quantitative one, as the maximal violation that could be attained in the CHSH inequality we construct is directly related to the unsharpness that must be required to two ±1-observables in order to be jointly measured. We also have derived a computable condition for two dichotomic generalized measurements to be simultaneously performed.

We have not been able to link our results to the previous existing works for the case of qubits. Even though finding how to derive their formulae from our results would not directly give any improvement, by studying how to do it we could possibly find a way to get algebraic characterizations beyond the qubit case by tring to extend the procedure.

More relationships and applications have later been found, such as that coexistence does not imply joint measurability [**109**], or the possibility of optimal steering [**94**].

We have also derived characterizations of joint measurability for more than two dichotomic observables, and for two observables with more than two outcomes. For more observables or outcomes a similar reduction to a CHSH-type inequality is not always possible, since by just considering pairwise incompatibility or grouping measurement outcomes we cannot capture the whole problem.

Uncle Hamiltonians for MPSs. The problem about the robustness of the parent Hamiltonian construction for Matrix Product States has been studied in almost full generality. We have constructed uncle Hamiltonians for both injective and block-injective MPSs, and studied its ground state space and spectrum for almost every perturbation: Whereas parent Hamiltonians are always gapped, uncle Hamiltonians are gapless, and they share their ground state space for block-injective MPSs.

The main consequence of these results stems on the role the spectral gap has for classification of matter into phases: depending on how we classify phases and the path of Hamiltonians we consider we can find the same states in the middle of a phase or in a phase transition. Even though some previous examples of states associated to different Hamiltonians with different spectral properties already existed, in this work we construct them sistematically for MPSs, and connect them with the lack of robustness of the parent Hamiltonian. Finally, uncle Hamiltonians can provide tools for finer classifications of states, in the direction of other works as [**13**].

Uncle Hamiltonians do not evidence any possible problem in numerical methods based on MPSs, since they start from a fixed Hamiltonian which does not change during the energy minimization process of such methods. However, for the inverse problem of having a given state and trying to find the interactions that made this state appear as a ground state by applying tomographic methods, uncle Hamiltonians show that the answer can be non-unique if one applies MPS methods.

We have only considered linear perturbations. For non-linear perturbations of the matrices, considering the linear approximations of the perturbations would yield the same results provided the uncle tensor is injective. When this is not the case, we could also consider higher-degree approximations in order to construct the uncle tensor.

One of the features that is worth studying is that, when the tensor description is perturbed, a leap on the entanglement entropy can be detected. This was already noted in two dimensions [**26**], and one can easily check that it also happens for GHZ spin chains.

This peculiarity may give more insight into the problem from the point of view of the states instead of from the point of view of the Hamiltonians we have taken.

Another related work we would like to study and connect to our results is [**52**], in which they provide a variatonal ansatz for excitations based on the MPS formalism, and which is closely related to the excitations we found to prove that the uncle Hamiltonians are gapless. A very interesting framework in terms of the tangent space of the manifold of MPSs is set in [**53**], and there exist other works studying the geometry of such manifold and its applications to numerical algorithms.

Uncle Hamiltonian for the toric code. In the case of two-dimensional lattices and Projective Entangled Pair States, the problem of describing which perturbations yield continuous changes in the parent Hamiltonians is far from being closed. We provide one example of a perturbation without this property, that can be easily generalized to other perturbations of the same PEPS and to other PEPSs – G- injective PEPSs –, in which the question is easily solved in terms of the symmetries of the perturbation [**26**]. The question of which perturbations are physical for generic PEPS seems to be more complicated, and a very interesting problem to study. In this direction, there is a candidate proposed in [**29**] of which perturbations should be considered natural.

The uncle Hamiltonian we have constructed for the toric code is an easy example of a gapless Hamiltonian for a topological ordered system, which are usually associated to gapped Hamiltonians. This construction has implications on the study of phases of matter, because of the role the spectral gap has in this problem, supporting the need to classify phases considering both ground states and Hamiltonians.

As we said before, uncle Hamiltonians can be easily provided for other G-injective PEPSs. For $\mathbb{Z}_2$-injective PEPSs – among which we would like to highlight the Resonating Valence Bond States, lately found to be within this class [**116**] – we would have a very similar construction. The uncle Hamiltonian would have the same ground space as the parent Hamiltonian, and it would be gapless. However, it is not that clear that we could claim that the spectrum is the complete positive real line when both lattice dimensions are allowed to grow indefinitely. For proving that fact we relied on the $\mathbb{Z}_2$-isometry of the PEPS for the toric code, and in the generic block-injective case for MPSs we used their normal form, which we are lacking now. For G-isometric PEPSs, one should be much more careful in proving the 'closure property' 6.4.2, which we found not very difficult thanks to our group being $\mathbb{Z}_2$; in this direction, we must note that the proof of the intersection property for parent Hamiltonians for G-injective PEPSs in [**114**] is not trivial at all.

Another problem which we have started addressing is the role of local/global symmetries in different levels for PEPSs. If one takes many copies of a G-injective PEPS, and then consider some symmetrization mapping among them, we get another PEPS as a result with the previous G-symmetry at each layer and another global symmetry among the different layers depending on the symmetrization mapping. That could provide new interesting topological models, due to the appearance of different anyonic excitations combining the anyons corresponding to each layer [**97**].

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